Full wwPDB X-ray Structure Validation Report (i)

May 17, 2020 – 01:16 am BST

PDB ID	:	4B3S
Title	:	Crystal structure of the 30S ribosome in complex with compound 37
Authors	:	Ng, C.L.; Lang, K.; Shcherbakov, D.; Matt, T.; Perez-Fernandez, D.; Patak, R.; Meyer, M.; Duscha, S.; Akbergenov, R.; Boukari, H.; Freihofer, P.; Kudyba, I.; Reddy, M.S.K.; Nandurikar, R.S.; Ramakrishnan, V.; Vasella, A.; Bottger, E.C.
Deposited on	:	2012-07-26
Resolution	:	3.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

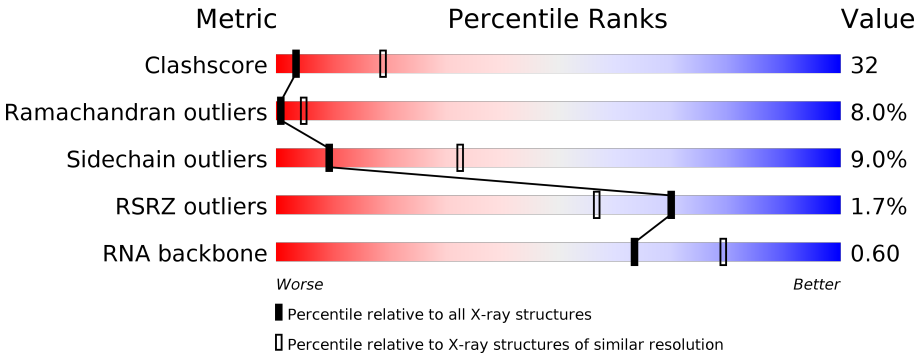
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)
RNA backbone	3102	1073 (3.50-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1521	% 34% 52% 11%
2	B	256	3% 25% 54% 11% 8%
3	C	239	21% 50% 14% 13%
4	D	208	3% 34% 55% 11%
5	E	161	37% 46% 10% 6%
6	F	101	33% 61% 6%

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Mol	Chain	Length	Quality of chain
7	G	155	3% 40% 55% 5%
8	H	138	49% 46% 6%
9	I	128	% 29% 62% 8%
10	J	104	9% 17% 57% 20% 5%
11	K	129	2% 47% 38% 8% 8%
12	L	132	3% 32% 48% 14% 5%
13	M	126	10% 24% 61% 14%
14	N	60	22% 65% 13%
15	O	88	% 49% 48%
16	P	88	44% 45% 6% 5%
17	Q	104	5% 36% 51% 13%
18	R	88	2% 25% 50% 6% 17%
19	S	92	% 23% 49% 14% 12%
20	T	106	34% 46% 13% 7%
21	V	26	8% 31% 54% 12%
22	W	6	17% 50% 33%
23	Z	16	44% 25% 19% 6% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	2552	-	-	-	X
24	MG	A	2554	-	-	-	X
24	MG	A	2597	-	-	-	X
24	MG	A	2608	-	-	-	X
24	MG	A	2613	-	-	-	X
24	MG	A	2626	-	-	-	X
24	MG	A	2631	-	-	-	X
24	MG	A	2645	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	2662	-	-	-	X
24	MG	A	2663	-	-	-	X
24	MG	A	2697	-	-	-	X
24	MG	A	2700	-	-	-	X
24	MG	L	1125	-	-	-	X
25	K	A	2680	-	-	-	X

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 52313 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1510	32446	14444	6006	10488	1508	0	0	0

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	235	1901	1213	342	341	5	0	0	1

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	207	1613	1016	315	281	1	0	0	1

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	208	1703	1066	339	291	7	0	0	0

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	151	1147	724	218	201	4	0	0	1

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	101	843	531	155	154	3	0	0	0

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	0	0	0
			1011	639	198	174			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	57	ARG	HIS	conflict	UNP P80374

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	95	GLN	GLU	conflict	UNP Q5SHP7

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	73	Total	C	N	O	0	0	0
			597	380	118	99			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	45	GLY	ALA	conflict	UNP Q5SLQ0

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	1
			648	414	120	112	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	34	VAL	ILE	conflict	UNP P80380

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	V	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called 5'-R(*UP*UP*CP*AP*AP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	W	4	Total	C	N	O	P	0	0	0
			79	37	12	27	3			

- Molecule 23 is a RNA chain called 5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*AP*AP*UP*CP*CP*CP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Z	15	Total	C	N	O	P	0	0	0
			319	144	60	101	14			

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	K	2	Total	Mg	0	0
			2	2		
24	E	1	Total	Mg	0	0
			1	1		

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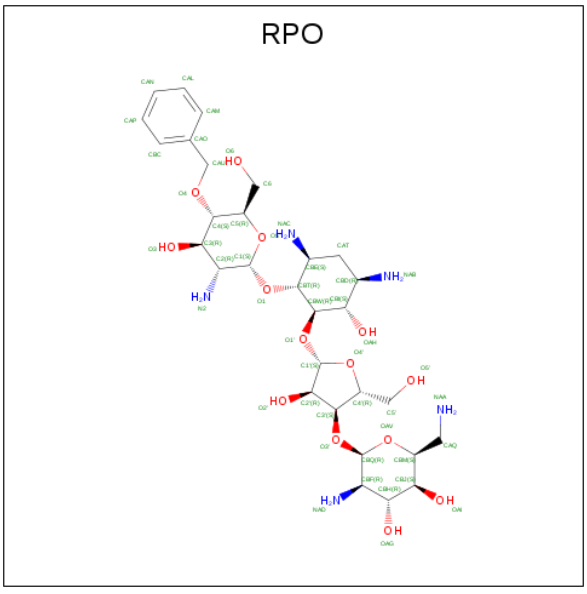
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	H	1	Total Mg 1 1	0	0
24	B	1	Total Mg 1 1	0	0
24	A	156	Total Mg 156 156	0	0
24	T	1	Total Mg 1 1	0	0
24	L	2	Total Mg 2 2	0	0
24	F	1	Total Mg 1 1	0	0
24	M	1	Total Mg 1 1	0	0

- Molecule 25 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	13	Total K 13 13	0	0

- Molecule 26 is (1R,2R,3S,4R,6S)-4,6-diamino-2-{[3-O-(2,6-diamino-2,6-dideoxy-beta-L-idopyranosyl)-beta-D-ribofuranosyl]oxy}-3-hydroxycyclohexyl 2-amino-4-O-benzyl-2-deoxy-alpha-D-glucopyranoside (three-letter code: RPO) (formula: $C_{30}H_{51}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	N	O	0	0
			49	30	5	14		

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

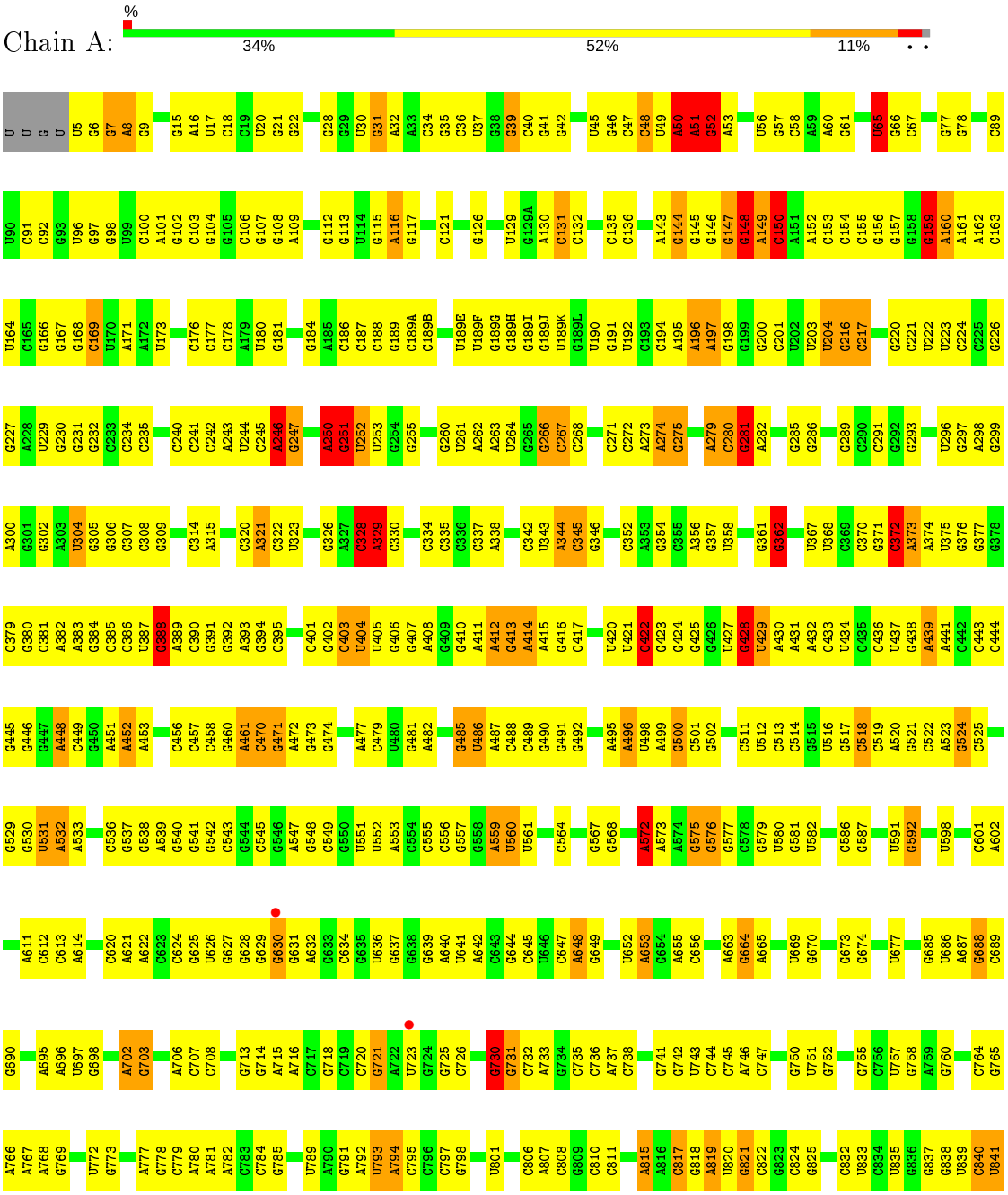
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	D	1	Total	Zn	0	0
			1	1		
27	N	1	Total	Zn	0	0
			1	1		

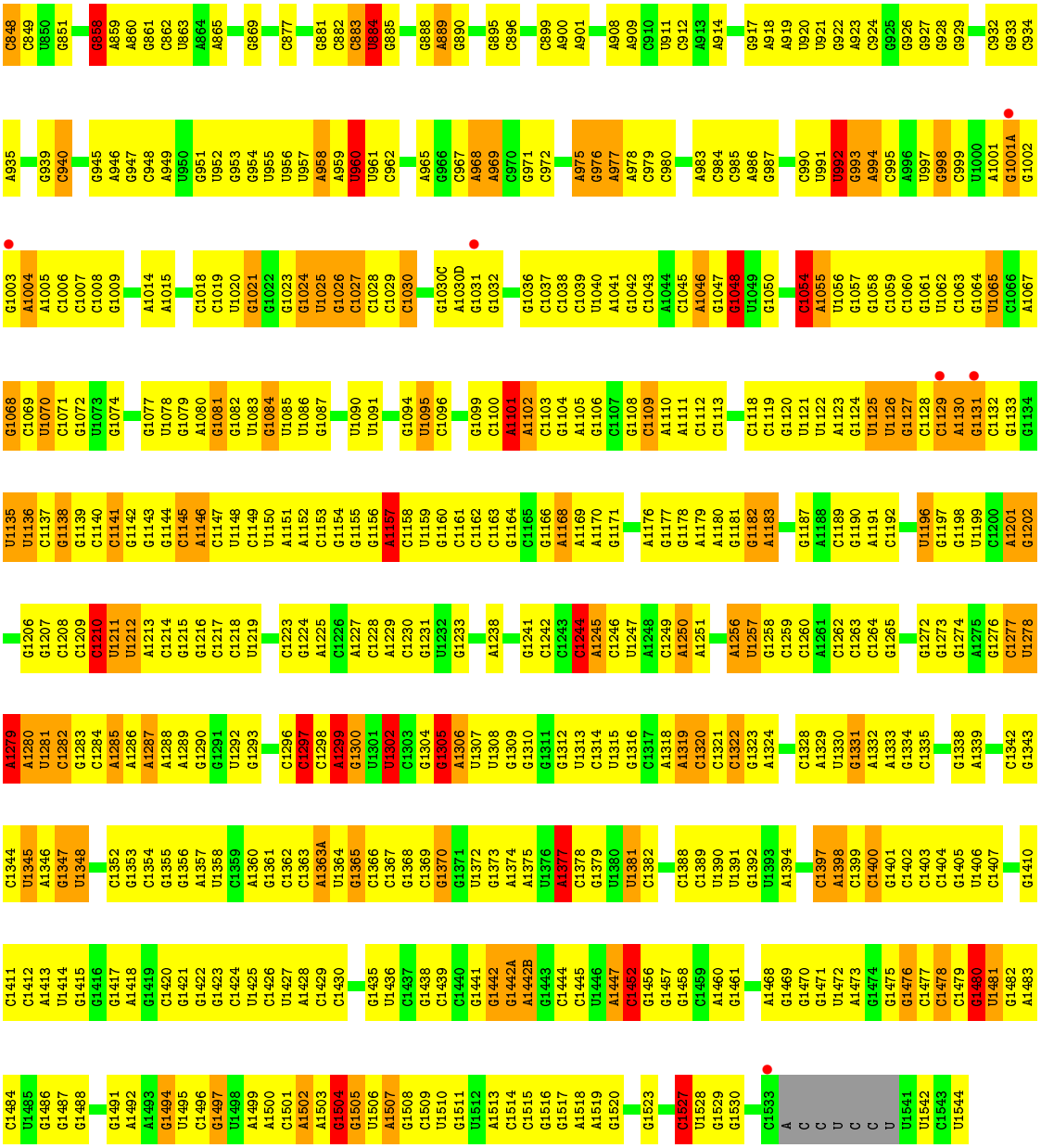
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 16S RIBOSOMAL RNA

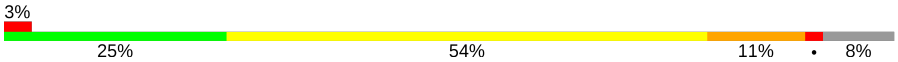
Chain A:

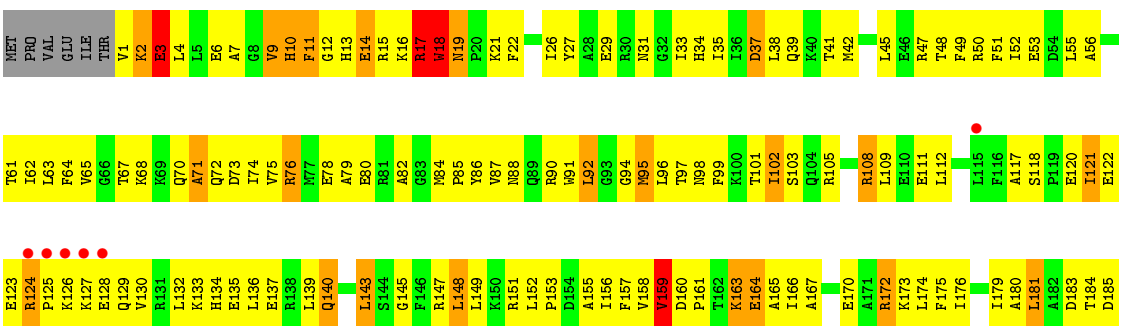


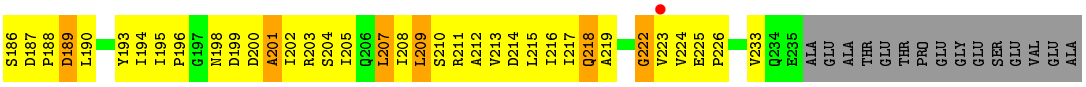


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain B:

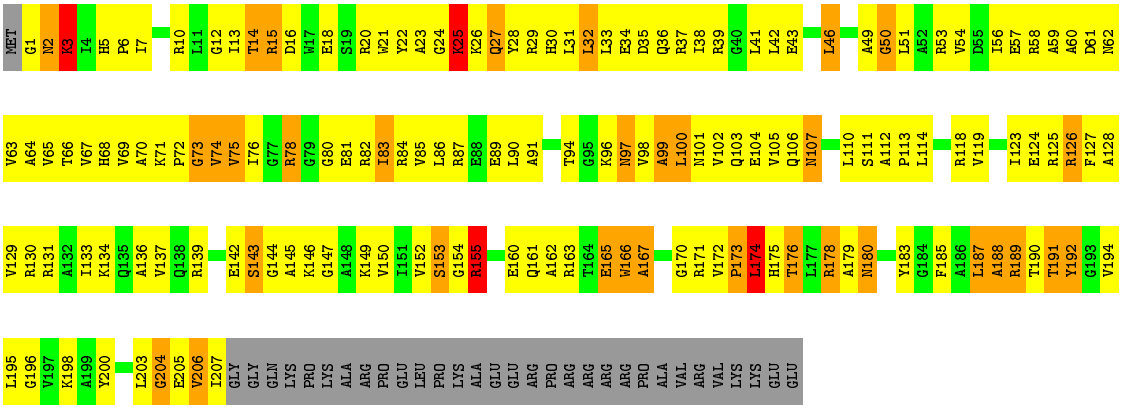






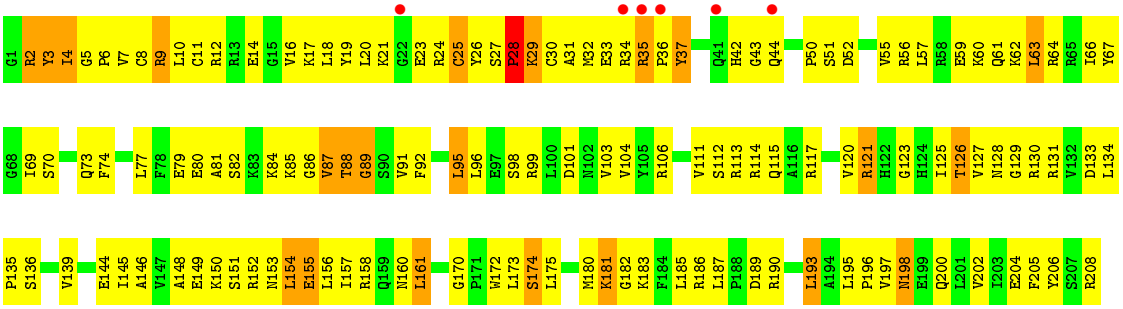
- Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain C:



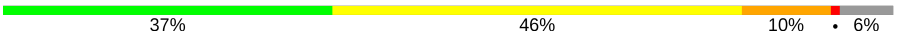
- Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain D:



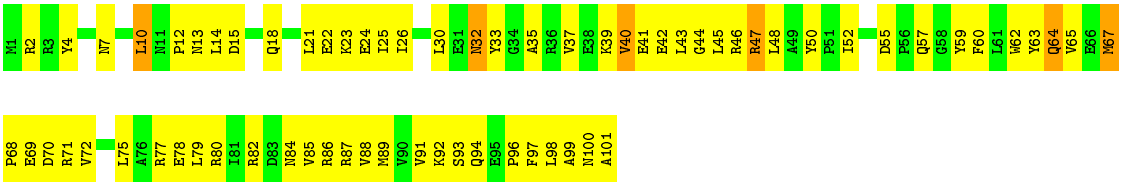
- Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain E:



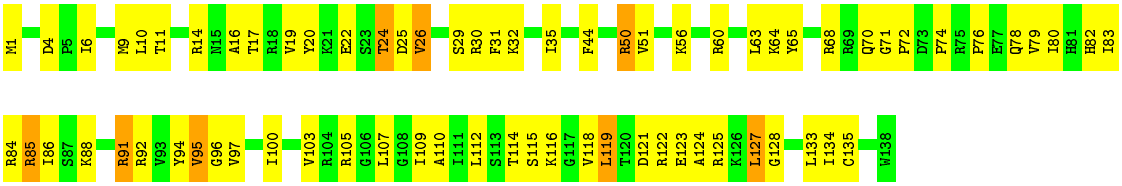
- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain F:

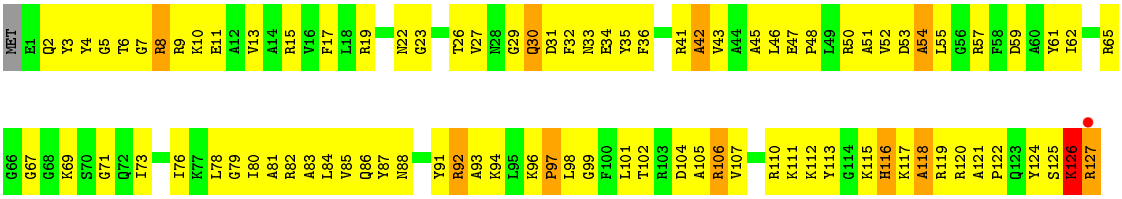


• Molecule 7: 30S RIBOSOMAL PROTEIN S7

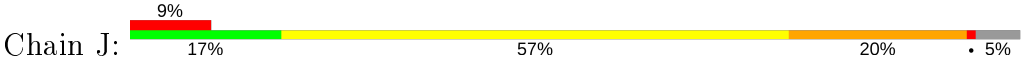
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

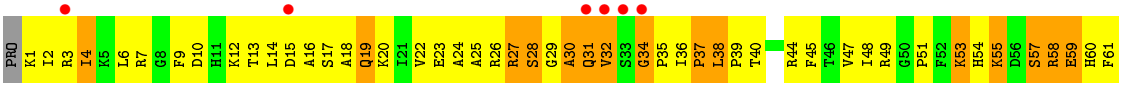


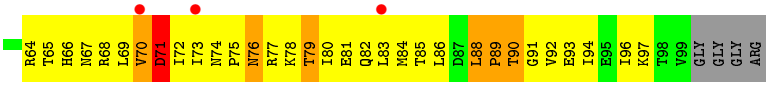
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



• Molecule 10: 30S RIBOSOMAL PROTEIN S10

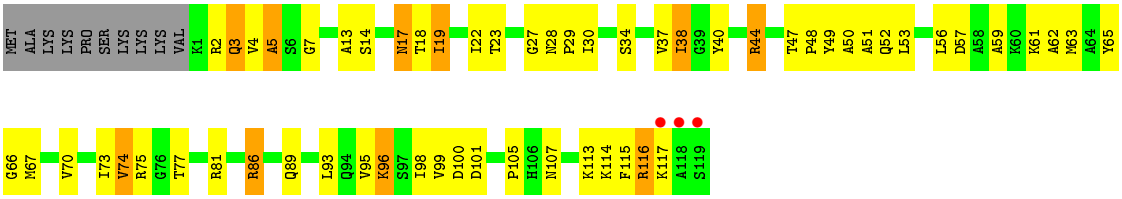






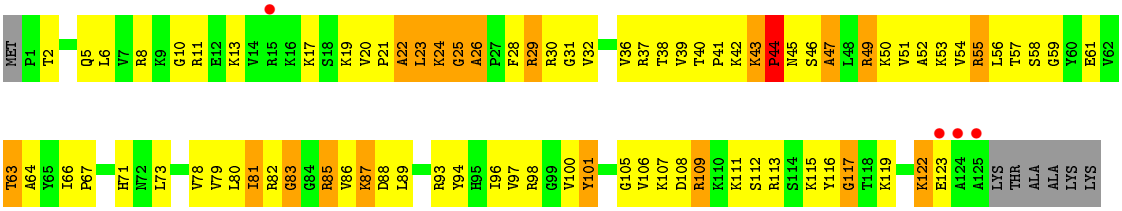
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain K:



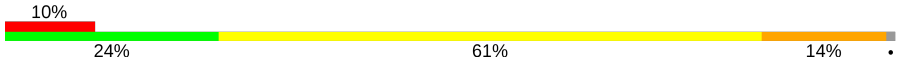
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

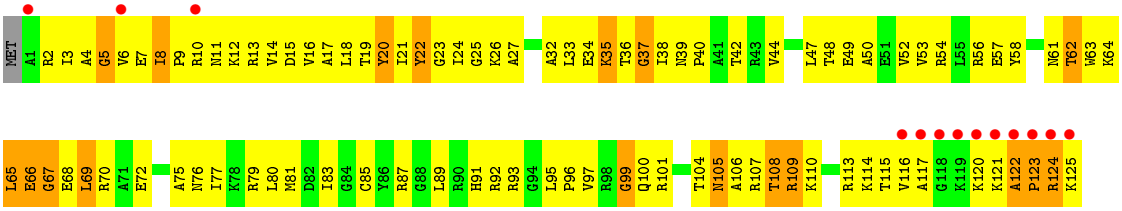
Chain L:



- Molecule 13: 30S RIBOSOMAL PROTEIN S13

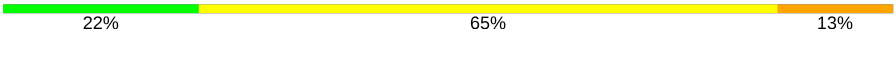
Chain M:

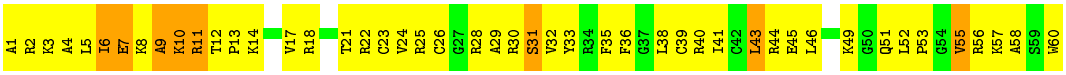




- Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

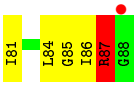
Chain N:





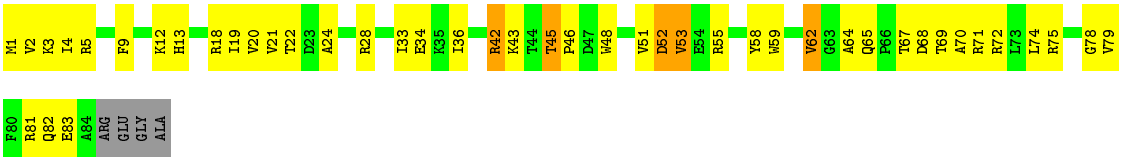
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain O:



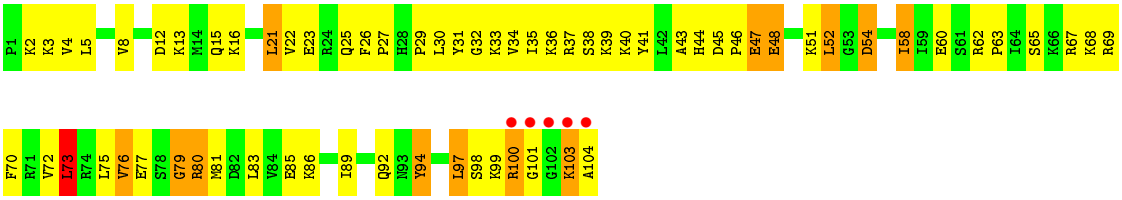
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain P:



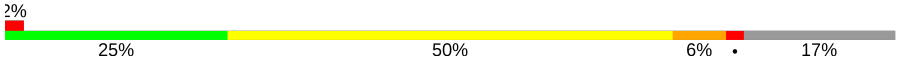
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

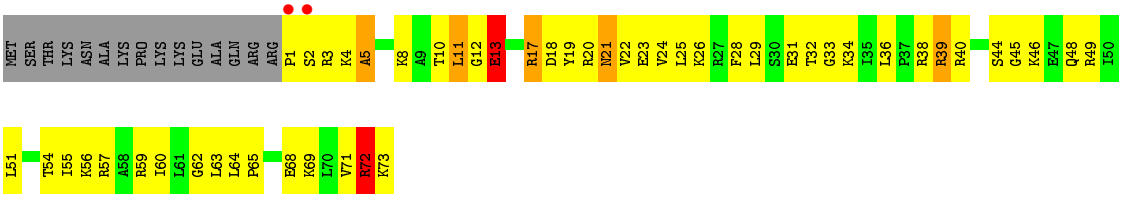
Chain Q:



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

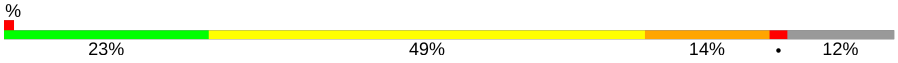
Chain R:

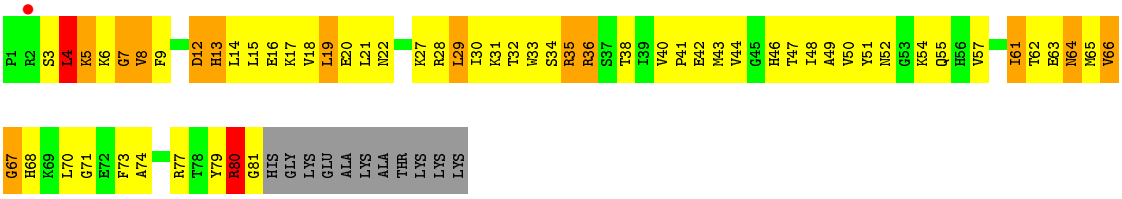




• Molecule 19: 30S RIBOSOMAL PROTEIN S19

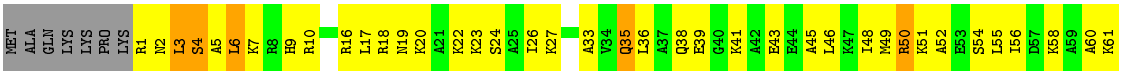
Chain S:





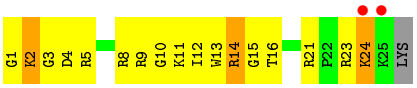
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain T:



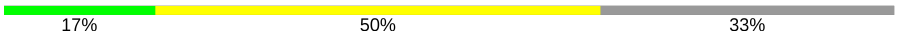
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

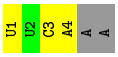
Chain V:



• Molecule 22: 5'-R(*UP*UP*CP*AP*AP*AP)-3'

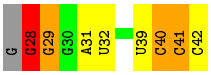
Chain W:





• Molecule 23: 5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*AP*AP*UP*CP*CP*CP)-3'

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	401.15Å 401.15Å 173.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.15 39.65 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.3 (40.00-3.15) 99.3 (39.65-3.15)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 3.12Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.210 , 0.247 0.215 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	75.6	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 83.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	52313	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, MG, ZN, RPO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.49	2/36318 (0.0%)	0.76	57/56682 (0.1%)
2	B	0.38	0/1936	0.66	0/2611
3	C	0.41	0/1637	0.67	0/2207
4	D	0.40	0/1733	0.64	0/2318
5	E	0.46	0/1163	0.71	0/1566
6	F	0.37	0/856	0.62	0/1154
7	G	0.38	0/1276	0.60	0/1709
8	H	0.44	0/1136	0.77	1/1527 (0.1%)
9	I	0.39	0/1029	0.67	0/1378
10	J	0.40	0/808	0.67	0/1087
11	K	0.40	0/900	0.72	1/1213 (0.1%)
12	L	0.47	0/987	0.80	1/1322 (0.1%)
13	M	0.37	0/1008	0.68	0/1347
14	N	0.46	0/501	0.71	0/664
15	O	0.38	0/745	0.65	1/992 (0.1%)
16	P	0.44	0/717	0.76	0/965
17	Q	0.43	0/870	0.74	0/1159
18	R	0.36	0/603	0.64	0/799
19	S	0.42	0/662	0.67	0/892
20	T	0.42	0/764	0.71	0/1006
21	V	0.50	0/213	0.61	0/279
22	W	0.58	0/87	0.93	1/133 (0.8%)
23	Z	0.42	0/357	0.76	1/555 (0.2%)
All	All	0.46	2/56306 (0.0%)	0.74	63/83565 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	36	29
23	Z	1	0
All	All	37	29

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	858	G	C5-C6	-9.69	1.32	1.42
1	A	858	G	C6-O6	-6.28	1.18	1.24

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1480	G	N9-C1'-C2'	10.00	127.00	114.00
1	A	250	A	C5'-C4'-O4'	9.98	121.08	109.10
1	A	884	U	C2'-C3'-O3'	9.87	131.21	109.50
1	A	281	G	C2'-C3'-O3'	9.50	130.41	109.50
1	A	992	U	C5'-C4'-C3'	9.40	131.03	116.00
1	A	65	U	C2'-C3'-O3'	9.33	130.03	109.50
1	A	1452	C	C2'-C3'-O3'	8.89	129.06	109.50
1	A	1210	C	N1-C1'-C2'	8.59	125.17	114.00
1	A	329	A	N9-C1'-C2'	8.40	124.91	114.00
23	Z	28	G	N9-C1'-C2'	8.37	124.89	114.00
1	A	250	A	C5'-C4'-C3'	8.36	129.38	116.00
1	A	992	U	C5'-C4'-O4'	8.35	119.11	109.10
1	A	730	G	C2'-C3'-O3'	7.72	126.49	109.50
1	A	50	A	N9-C1'-C2'	7.53	123.79	114.00
1	A	1305	G	N9-C1'-C2'	7.47	123.71	114.00
1	A	159	G	N9-C1'-C2'	7.44	123.67	114.00
1	A	246	A	C2'-C3'-O3'	7.43	125.85	109.50
1	A	250	A	N9-C1'-C2'	7.37	123.58	114.00
1	A	1157	A	N9-C1'-C2'	7.36	123.57	114.00
1	A	1297	C	C2'-C3'-O3'	7.27	125.49	109.50
1	A	1480	G	C2'-C3'-O3'	7.20	125.33	109.50
1	A	1502	A	N9-C1'-C2'	7.19	123.35	114.00
1	A	329	A	C5'-C4'-O4'	7.19	117.72	109.10
1	A	1054	C	C2'-C3'-O3'	7.13	125.19	109.50
1	A	159	G	C2'-C3'-O3'	7.05	125.00	109.50
1	A	372	C	C2'-C3'-O3'	7.04	124.99	109.50
1	A	1210	C	C2'-C3'-O3'	7.02	124.94	109.50
1	A	304	U	C2'-C3'-O3'	7.01	124.92	109.50
1	A	196	A	C2'-C3'-O3'	7.00	124.91	109.50
1	A	992	U	N1-C1'-C2'	7.00	123.09	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1377	A	C2'-C3'-O3'	6.99	124.89	113.70
1	A	1101	A	C2'-C3'-O3'	6.97	124.85	113.70
1	A	572	A	C2'-C3'-O3'	6.95	124.82	113.70
1	A	1527	C	C5'-C4'-C3'	-6.90	104.96	116.00
1	A	1084	G	C2'-C3'-O3'	6.55	124.19	113.70
1	A	148	G	C2'-C3'-O3'	6.52	124.14	113.70
1	A	1299	A	N9-C1'-C2'	6.41	122.33	114.00
1	A	328	C	N1-C1'-C2'	6.31	122.20	114.00
1	A	968	A	C2'-C3'-O3'	6.29	123.77	113.70
1	A	1210	C	C5'-C4'-O4'	6.13	116.45	109.10
1	A	1305	G	C2'-C3'-O3'	6.09	123.44	113.70
1	A	960	U	N1-C1'-C2'	5.89	121.66	114.00
1	A	51	A	N9-C1'-C2'	5.87	121.63	114.00
1	A	428	G	C2'-C3'-O3'	5.82	123.02	113.70
15	O	44	VAL	N-CA-C	-5.82	95.29	111.00
1	A	246	A	C4'-C3'-O3'	5.80	124.61	113.00
1	A	362	G	C5'-C4'-O4'	-5.77	102.17	109.10
1	A	858	G	C6-C5-N7	-5.68	126.99	130.40
1	A	1504	G	C2'-C3'-O3'	5.67	122.77	113.70
1	A	251	G	C2'-C3'-O3'	5.65	122.75	113.70
12	L	22	ALA	N-CA-C	-5.61	95.84	111.00
1	A	52	G	C5'-C4'-C3'	5.60	124.96	116.00
11	K	27	GLY	N-CA-C	5.58	127.04	113.10
1	A	422	C	N1-C1'-C2'	5.45	121.08	114.00
1	A	1210	C	C5'-C4'-C3'	5.43	124.69	116.00
22	W	4	A	C2'-C3'-O3'	5.37	122.29	113.70
1	A	150	C	C5'-C4'-C3'	-5.20	107.68	116.00
8	H	96	GLY	N-CA-C	-5.14	100.24	113.10
1	A	559	A	C2'-C3'-O3'	5.11	121.87	113.70
1	A	858	G	O4'-C1'-N9	-5.10	104.12	108.20
1	A	1363	C	C5'-C4'-O4'	5.06	115.17	109.10
1	A	388	G	N9-C1'-C2'	5.05	120.56	114.00
1	A	1244	C	N1-C1'-C2'	-5.03	106.46	112.00

All (37) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	50	A	C4'
1	A	65	U	C3'
1	A	159	G	C4',C3',C1'
1	A	196	A	C3'
1	A	246	A	C3'

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Mol	Chain	Res	Type	Atom
1	A	250	A	C4',C1'
1	A	251	G	C4',C3',C1'
1	A	281	G	C3'
1	A	304	U	C3'
1	A	329	A	C4',C3',C1'
1	A	730	G	C3'
1	A	884	U	C3'
1	A	992	U	C4'
1	A	1084	G	C3'
1	A	1157	A	C4',C3',C1'
1	A	1210	C	C4',C3',C1'
1	A	1297	C	C4',C3'
1	A	1305	G	C4',C3'
1	A	1377	A	C3'
1	A	1452	C	C3'
1	A	1480	G	C4',C3',C1'
23	Z	28	G	C1'

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1048	G	Sidechain
1	A	1077	G	Sidechain
1	A	1081	G	Sidechain
1	A	1210	C	Sidechain
1	A	1244	C	Sidechain
1	A	1279	A	Sidechain
1	A	1299	A	Sidechain
1	A	1302	U	Sidechain
1	A	1331	G	Sidechain
1	A	1339	A	Sidechain
1	A	1345	U	Sidechain
1	A	1401	G	Sidechain
1	A	1528	U	Sidechain
1	A	159	G	Sidechain
1	A	253	U	Sidechain
1	A	291	C	Sidechain
1	A	297	G	Sidechain
1	A	380	G	Sidechain
1	A	404	U	Sidechain
1	A	51	A	Sidechain
1	A	529	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	560	U	Sidechain
1	A	561	U	Sidechain
1	A	592	G	Sidechain
1	A	611	A	Sidechain
1	A	664	G	Sidechain
1	A	858	G	Sidechain
1	A	883	C	Sidechain
1	A	940	C	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32446	0	16381	1028	0
2	B	1901	0	1954	225	0
3	C	1613	0	1680	211	0
4	D	1703	0	1766	171	0
5	E	1147	0	1210	111	0
6	F	843	0	857	87	0
7	G	1257	0	1299	79	0
8	H	1116	0	1177	95	0
9	I	1011	0	1046	109	0
10	J	795	0	843	146	0
11	K	885	0	907	78	0
12	L	971	0	1059	108	0
13	M	997	0	1075	121	0
14	N	492	0	532	76	0
15	O	734	0	773	48	0
16	P	701	0	720	49	0
17	Q	857	0	932	76	0
18	R	597	0	670	84	0
19	S	648	0	675	86	0
20	T	762	0	862	79	0
21	V	209	0	224	32	0
22	W	79	0	44	2	0
23	Z	319	0	164	11	0
24	A	156	0	0	0	0
24	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	E	1	0	0	0	0
24	F	1	0	0	0	0
24	H	1	0	0	0	0
24	K	2	0	0	0	0
24	L	2	0	0	0	0
24	M	1	0	0	0	0
24	T	1	0	0	0	0
25	A	13	0	0	0	0
26	A	49	0	51	6	0
27	D	1	0	0	0	0
27	N	1	0	0	0	0
All	All	52313	0	36901	2845	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (2845) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:G:H2'	1:A:362:G:H5"	1.27	1.12
3:C:25:LYS:H	3:C:25:LYS:HD3	1.09	1.12
12:L:43:LYS:HB3	12:L:44:PRO:HD3	1.30	1.11
1:A:402:G:H2'	1:A:403:C:H5"	1.26	1.11
3:C:190:THR:HG22	3:C:191:THR:H	1.11	1.10
1:A:1029:C:H2'	1:A:1030:C:H5"	1.31	1.10
8:H:86:ILE:HG21	8:H:133:LEU:HD23	1.32	1.09
4:D:82:SER:HA	4:D:88:THR:HG21	1.12	1.08
7:G:53:THR:HG22	7:G:55:GLN:H	1.13	1.08
16:P:74:LEU:HG	16:P:79:VAL:HG21	1.36	1.07
1:A:1130:A:H5'	1:A:1131:G:C5'	1.84	1.07
19:S:32:THR:HG22	19:S:34:SER:H	1.20	1.07
2:B:9:VAL:HG13	2:B:203:ARG:HG3	1.36	1.06
12:L:83:GLY:HA2	12:L:94:TYR:HA	1.36	1.06
2:B:78:GLU:HB3	2:B:213:VAL:HG21	1.39	1.05
10:J:25:ALA:HB2	10:J:83:LEU:HD11	1.37	1.04
11:K:96:LYS:HE2	11:K:96:LYS:HA	1.34	1.04
10:J:36:ILE:HD12	10:J:69:LEU:HD23	1.38	1.04
19:S:21:LEU:HD13	19:S:27:LYS:HD2	1.39	1.03
1:A:146:G:H2'	1:A:147:G:H5"	1.41	1.03
1:A:1130:A:C5'	1:A:1131:G:H5"	1.88	1.02
12:L:37:ARG:HG2	12:L:38:THR:H	1.23	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:79:VAL:HG21	12:L:96:ILE:HG23	1.42	1.01
1:A:647:C:H2'	1:A:648:A:H5"	1.36	1.00
1:A:839:U:H3'	1:A:840:C:H5"	1.42	1.00
1:A:1479:C:H2'	1:A:1480:G:H5"	1.43	1.00
3:C:90:LEU:HD12	3:C:91:ALA:N	1.75	1.00
12:L:43:LYS:HB3	12:L:44:PRO:CD	1.90	1.00
1:A:1086:U:H3	1:A:1099:G:H22	1.09	1.00
1:A:1130:A:H5'	1:A:1131:G:H5"	1.00	1.00
3:C:63:VAL:HB	3:C:98:VAL:HB	1.44	1.00
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.44	0.99
13:M:9:PRO:HB2	13:M:17:ALA:HB1	1.41	0.99
1:A:522:C:H41	12:L:49:ARG:HH22	1.10	0.99
1:A:647:C:C2'	1:A:648:A:H5"	1.93	0.98
2:B:71:ALA:HB2	2:B:205:ILE:HD13	1.46	0.98
4:D:82:SER:HA	4:D:88:THR:CG2	1.92	0.98
1:A:135:C:O2	16:P:1:MET:HB2	1.63	0.98
1:A:1276:G:H3'	1:A:1277:C:H5"	1.44	0.97
2:B:1:VAL:HG21	2:B:215:LEU:HD23	1.45	0.97
10:J:29:GLY:HA2	10:J:76:ASN:ND2	1.79	0.96
1:A:146:G:C2'	1:A:147:G:H5"	1.95	0.96
1:A:1502:A:H2	1:A:1505:G:H1	1.10	0.96
12:L:85:ARG:HH21	12:L:93:ARG:HE	1.14	0.95
3:C:27:GLN:HA	3:C:30:HIS:HD2	1.29	0.95
3:C:76:ILE:HA	3:C:83:ILE:HB	1.47	0.95
1:A:361:G:C2'	1:A:362:G:H5"	1.96	0.94
5:E:87:LEU:HD23	5:E:116:THR:HG22	1.47	0.94
11:K:114:LYS:HE3	11:K:115:PHE:HE1	1.31	0.94
1:A:1020:U:H2'	1:A:1021:G:H5"	1.49	0.94
1:A:1045:C:H2'	1:A:1046:A:H5"	1.48	0.94
11:K:44:ARG:O	11:K:47:THR:HG22	1.66	0.94
1:A:460:G:H3'	1:A:461:A:C5'	1.99	0.93
1:A:953:G:H1'	13:M:124:ARG:HA	1.49	0.93
3:C:13:ILE:HG22	3:C:14:THR:H	1.31	0.93
1:A:402:G:C2'	1:A:403:C:H5"	1.98	0.93
1:A:922:G:H4'	5:E:16:GLN:HA	1.50	0.92
5:E:78:VAL:HG12	5:E:85:ILE:HG22	1.48	0.92
1:A:371:G:O2'	1:A:372:C:H5'	1.69	0.92
10:J:30:ALA:HB2	10:J:74:ASN:ND2	1.85	0.91
4:D:104:VAL:HG21	4:D:125:ILE:HD13	1.51	0.91
3:C:190:THR:HG22	3:C:191:THR:N	1.85	0.91
12:L:71:HIS:HD2	12:L:73:LEU:H	1.16	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1029:C:C2'	1:A:1030:C:H5"	2.01	0.90
11:K:77:THR:HG23	11:K:81:ARG:HH21	1.35	0.90
13:M:14:VAL:HG21	13:M:47:LEU:HD21	1.53	0.90
3:C:173:PRO:HB2	3:C:176:THR:HG23	1.54	0.90
13:M:36:THR:HG22	13:M:38:ILE:HD11	1.54	0.90
12:L:41:PRO:HG3	12:L:49:ARG:HD3	1.54	0.90
1:A:1182:G:H4'	1:A:1183:A:H5'	1.53	0.89
9:I:43:VAL:HG12	9:I:50:ARG:HH12	1.34	0.89
12:L:23:LEU:O	12:L:25:GLY:N	2.06	0.88
17:Q:94:TYR:HA	17:Q:97:LEU:HD11	1.55	0.88
13:M:48:THR:HG22	13:M:50:ALA:H	1.38	0.88
5:E:70:GLY:HA3	5:E:112:THR:HG22	1.55	0.88
10:J:30:ALA:HB2	10:J:74:ASN:HD22	1.38	0.88
15:O:25:GLU:OE2	15:O:76:ARG:HD2	1.72	0.88
14:N:56:ARG:HG2	14:N:57:LYS:H	1.35	0.88
3:C:31:LEU:O	3:C:35:ASP:HB2	1.74	0.88
4:D:37:TYR:HD1	4:D:37:TYR:H	1.17	0.88
1:A:939:G:H5"	7:G:101:ARG:NH2	1.89	0.88
9:I:105:ALA:O	9:I:107:VAL:HG23	1.73	0.87
10:J:17:SER:HA	10:J:20:LYS:HE2	1.55	0.87
1:A:251:G:H2'	1:A:252:U:H5"	1.57	0.87
12:L:71:HIS:HA	12:L:98:ARG:HH22	1.39	0.87
1:A:451:A:H61	1:A:481:G:H5'	1.38	0.86
3:C:107:ASN:HD22	3:C:110:LEU:HG	1.39	0.86
11:K:99:VAL:HG22	18:R:71:VAL:HA	1.57	0.86
4:D:61:GLN:HE22	4:D:64:ARG:HH12	1.21	0.86
1:A:1060:C:C5	3:C:1:GLY:HA3	2.10	0.86
1:A:1128:C:O2'	1:A:1129:C:H5"	1.75	0.86
14:N:26:CYS:SG	14:N:28:ARG:HB2	2.16	0.86
1:A:1284:C:H3'	1:A:1285:A:H5"	1.58	0.85
4:D:208:ARG:HB3	4:D:208:ARG:NH1	1.91	0.85
4:D:61:GLN:HE22	4:D:64:ARG:NH1	1.74	0.85
12:L:51:VAL:HG12	12:L:52:ALA:H	1.41	0.85
6:F:25:ILE:HD12	6:F:25:ILE:H	1.40	0.85
10:J:6:LEU:CD1	10:J:18:ALA:HB2	2.06	0.85
1:A:1399:C:H4'	1:A:1400:C:H5"	1.56	0.84
6:F:101:ALA:HA	18:R:13:GLU:OE1	1.76	0.84
1:A:1108:G:H2'	1:A:1109:C:H5"	1.58	0.84
1:A:1190:G:OP1	3:C:3:LYS:HA	1.77	0.84
10:J:27:ARG:HH11	10:J:27:ARG:HB2	1.41	0.84
1:A:168:G:H2'	1:A:169:C:H5"	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1366:C:H2'	1:A:1367:C:C6	2.13	0.84
2:B:160:ASP:HB2	2:B:199:ASP:HB2	1.60	0.84
11:K:17:ASN:HD22	11:K:18:THR:N	1.75	0.84
1:A:1038:C:H2'	1:A:1039:C:H6	1.43	0.84
12:L:30:ARG:O	12:L:57:THR:HG23	1.77	0.84
5:E:39:LEU:HD11	5:E:128:ALA:HB1	1.60	0.83
8:H:24:THR:HG22	8:H:63:LEU:HD21	1.60	0.83
11:K:114:LYS:HE3	11:K:115:PHE:CE1	2.14	0.83
13:M:116:VAL:HG12	13:M:117:ALA:H	1.43	0.83
19:S:36:ARG:H	19:S:36:ARG:HD2	1.41	0.83
1:A:1502:A:H2	1:A:1505:G:N1	1.76	0.83
9:I:7:GLY:HA2	9:I:78:LEU:HD12	1.58	0.83
1:A:168:G:C2'	1:A:169:C:H5"	2.08	0.83
2:B:65:VAL:HB	2:B:158:VAL:HG12	1.59	0.83
1:A:1321:C:H3'	1:A:1322:C:H5"	1.60	0.82
10:J:10:ASP:O	10:J:13:THR:HG22	1.79	0.82
12:L:51:VAL:HG12	12:L:52:ALA:N	1.94	0.82
11:K:17:ASN:HD22	11:K:18:THR:H	1.23	0.82
6:F:47:ARG:HE	6:F:47:ARG:N	1.77	0.82
3:C:69:VAL:HG12	3:C:71:LYS:H	1.43	0.82
1:A:647:C:H2'	1:A:648:A:C5'	2.09	0.82
11:K:81:ARG:CZ	18:R:73:LYS:HE2	2.09	0.82
1:A:180:U:H2'	1:A:181:G:H5'	1.62	0.82
5:E:123:ASN:HD22	5:E:124:PRO:HD2	1.44	0.81
13:M:14:VAL:HG23	13:M:42:THR:O	1.80	0.81
17:Q:3:LYS:HD2	17:Q:5:LEU:HD21	1.61	0.81
1:A:858:G:H8	1:A:858:G:C5'	1.93	0.81
1:A:969:A:H61	13:M:125:LYS:HG3	1.44	0.81
2:B:207:LEU:HD22	2:B:208:ILE:HD13	1.62	0.81
1:A:858:G:C6	1:A:869:G:N7	2.48	0.81
12:L:37:ARG:HH22	12:L:53:LYS:NZ	1.78	0.81
3:C:25:LYS:N	3:C:25:LYS:HD3	1.94	0.81
10:J:1:LYS:HG2	10:J:73:ILE:HG23	1.62	0.81
15:O:52:HIS:CE1	15:O:56:LEU:HD13	2.16	0.81
3:C:190:THR:CG2	3:C:191:THR:H	1.91	0.80
2:B:124:ARG:HH22	3:C:178:ARG:HH12	1.28	0.80
13:M:39:ASN:O	13:M:42:THR:HG23	1.81	0.80
15:O:52:HIS:HE1	15:O:56:LEU:HD13	1.44	0.80
1:A:1472:U:H2'	1:A:1473:A:O4'	1.81	0.80
12:L:43:LYS:CB	12:L:44:PRO:HD3	2.10	0.80
15:O:86:ILE:O	15:O:87:ARG:HB2	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:106:LEU:HD13	5:E:114:ILE:HG21	1.63	0.80
2:B:53:GLU:HB3	2:B:215:LEU:HD11	1.63	0.80
1:A:1020:U:C2'	1:A:1021:G:H5"	2.12	0.80
1:A:1024:G:O2'	1:A:1025:U:H5'	1.80	0.80
8:H:56:LYS:HD2	8:H:56:LYS:H	1.46	0.80
1:A:1201:A:H4'	1:A:1202:G:O5'	1.82	0.80
1:A:718:G:H5'	11:K:107:ASN:HD22	1.47	0.80
11:K:59:ALA:HB1	11:K:93:LEU:HD12	1.62	0.80
1:A:613:C:O2'	1:A:614:A:H5'	1.83	0.79
2:B:126:LYS:HA	2:B:129:GLN:HB2	1.63	0.79
7:G:68:VAL:HG11	7:G:133:ALA:HB1	1.61	0.79
1:A:580:U:H2'	1:A:581:G:O4'	1.82	0.79
4:D:150:LYS:H	4:D:150:LYS:HD2	1.47	0.79
1:A:357:G:O2'	1:A:358:U:H5'	1.83	0.79
1:A:489:C:H2'	1:A:490:G:H8	1.48	0.79
1:A:1282:C:H5'	1:A:1282:C:C6	2.17	0.79
4:D:161:LEU:HD13	4:D:180:MET:HG2	1.65	0.78
4:D:173:LEU:O	4:D:185:LEU:HG	1.83	0.78
4:D:35:ARG:HA	4:D:37:TYR:HE1	1.47	0.78
5:E:101:VAL:HB	5:E:102:PRO:HD3	1.64	0.78
7:G:112:GLU:HG2	7:G:118:ARG:HG2	1.64	0.78
13:M:49:GLU:O	13:M:53:VAL:HG23	1.83	0.78
1:A:1367:C:H5'	10:J:58:ARG:HH21	1.47	0.78
17:Q:52:LEU:HD12	17:Q:52:LEU:H	1.48	0.78
6:F:100:ASN:HD22	18:R:8:LYS:HG2	1.47	0.78
1:A:1435:G:H2'	1:A:1436:U:C6	2.18	0.78
1:A:386:C:C2'	1:A:387:U:H5'	2.12	0.78
3:C:57:GLU:H	3:C:64:ALA:HB3	1.47	0.78
20:T:38:GLN:HB2	20:T:84:LEU:HD13	1.65	0.78
3:C:18:GLU:HG2	3:C:53:ARG:HD2	1.66	0.78
2:B:108:ARG:HH21	2:B:112:LEU:HG	1.49	0.78
1:A:1425:U:H2'	1:A:1426:C:H6	1.49	0.78
1:A:362:G:H8	1:A:362:G:H5'	1.49	0.78
8:H:116:LYS:HD3	8:H:127:LEU:HD12	1.64	0.78
2:B:10:HIS:HB2	2:B:198:ASN:OD1	1.83	0.78
19:S:64:ASN:HD22	19:S:65:MET:N	1.82	0.78
1:A:1391:U:H2'	1:A:1392:G:C8	2.19	0.77
1:A:1038:C:H2'	1:A:1039:C:C6	2.19	0.77
3:C:130:ARG:NH1	3:C:130:ARG:HB2	1.99	0.77
10:J:85:THR:O	10:J:86:LEU:HD23	1.85	0.77
1:A:1144:G:H21	1:A:1146:A:H62	1.28	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:24:LYS:C	12:L:26:ALA:H	1.84	0.77
19:S:4:LEU:O	19:S:5:LYS:HB2	1.82	0.77
2:B:215:LEU:O	2:B:219:ALA:HB2	1.84	0.77
7:G:58:LEU:O	7:G:62:LYS:HG2	1.85	0.77
2:B:10:HIS:ND1	2:B:11:PHE:N	2.31	0.77
1:A:957:U:H3	1:A:960:U:H5"	1.47	0.77
2:B:71:ALA:HB2	2:B:205:ILE:CD1	2.15	0.77
6:F:48:LEU:HG	6:F:57:GLN:HA	1.65	0.77
12:L:42:LYS:HE3	12:L:43:LYS:HB2	1.67	0.77
10:J:82:GLN:O	10:J:86:LEU:HD12	1.84	0.77
10:J:47:VAL:HG13	14:N:40:ARG:HD2	1.66	0.77
5:E:11:ARG:HD3	5:E:22:PHE:HD2	1.49	0.77
5:E:11:ARG:HD3	5:E:22:PHE:CD2	2.19	0.76
5:E:14:ARG:HD3	5:E:21:ARG:HB2	1.67	0.76
1:A:706:A:O4'	11:K:19:ILE:HD11	1.86	0.76
13:M:61:ASN:O	13:M:62:THR:HB	1.84	0.76
21:V:5:ARG:HE	21:V:14:ARG:HH12	1.30	0.76
1:A:362:G:C8	1:A:362:G:H5'	2.20	0.76
1:A:939:G:H5"	7:G:101:ARG:HH22	1.50	0.76
5:E:123:ASN:HD22	5:E:124:PRO:CD	1.98	0.76
16:P:9:PHE:CD2	16:P:18:ARG:HG3	2.20	0.76
1:A:1425:U:H2'	1:A:1426:C:C6	2.21	0.76
1:A:1060:C:H5	3:C:1:GLY:HA3	1.51	0.76
8:H:56:LYS:N	8:H:56:LYS:HD2	2.00	0.76
1:A:371:G:C2'	1:A:372:C:H5'	2.16	0.76
3:C:90:LEU:HD12	3:C:91:ALA:H	1.48	0.76
4:D:82:SER:CA	4:D:88:THR:HG21	2.06	0.76
10:J:1:LYS:HA	10:J:73:ILE:HA	1.66	0.76
4:D:173:LEU:O	4:D:174:SER:HB3	1.85	0.76
19:S:63:GLU:O	19:S:66:VAL:HG23	1.84	0.76
10:J:55:LYS:HG2	10:J:58:ARG:HH12	1.47	0.76
17:Q:94:TYR:HA	17:Q:97:LEU:CD1	2.14	0.76
18:R:31:GLU:H	18:R:31:GLU:CD	1.89	0.76
1:A:653:A:H5'	8:H:56:LYS:HE3	1.67	0.76
2:B:2:LYS:O	2:B:3:GLU:HB2	1.85	0.76
4:D:2:ARG:HE	4:D:2:ARG:HA	1.50	0.76
2:B:118:SER:O	2:B:121:ILE:HG13	1.86	0.75
4:D:111:VAL:HG23	4:D:160:ASN:HD21	1.50	0.75
21:V:5:ARG:HG2	21:V:14:ARG:NH1	2.01	0.75
3:C:51:LEU:HD23	3:C:51:LEU:H	1.49	0.75
6:F:21:LEU:O	6:F:24:GLU:HB3	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1427:U:H3	1:A:1473:A:N6	1.84	0.75
20:T:67:LYS:HG3	20:T:68:ASN:H	1.52	0.75
8:H:9:MET:HG3	8:H:26:VAL:HG21	1.67	0.75
1:A:1343:G:H2'	1:A:1344:C:C6	2.22	0.75
1:A:888:G:H3'	1:A:889:A:H5"	1.69	0.75
1:A:1412:C:H2'	1:A:1413:A:C8	2.20	0.75
2:B:50:ARG:HH11	2:B:50:ARG:HB2	1.50	0.75
4:D:154:LEU:HB3	4:D:157:ILE:HD13	1.68	0.75
1:A:946:A:H2'	1:A:947:G:C8	2.22	0.75
2:B:149:LEU:HD21	2:B:153:PRO:HD3	1.69	0.75
1:A:1210:C:H4'	1:A:1211:U:OP2	1.87	0.74
1:A:1330:U:H2'	1:A:1331:G:H5'	1.66	0.74
4:D:25:CYS:HA	4:D:30:CYS:HB2	1.69	0.74
17:Q:77:GLU:CD	17:Q:80:ARG:HD2	2.07	0.74
1:A:146:G:C3'	1:A:147:G:H5"	2.17	0.74
1:A:948:C:OP1	13:M:108:THR:HG22	1.87	0.74
1:A:993:G:H4'	1:A:994:A:OP2	1.85	0.74
12:L:79:VAL:CG2	12:L:96:ILE:HG23	2.16	0.74
18:R:71:VAL:O	18:R:72:ARG:HB2	1.85	0.74
1:A:1305:G:H5"	21:V:3:GLY:HA3	1.67	0.74
1:A:279:A:H8	1:A:279:A:H5'	1.50	0.74
1:A:738:C:H5"	6:F:69:GLU:HB3	1.68	0.74
12:L:51:VAL:HG11	12:L:63:THR:HG22	1.69	0.74
4:D:156:LEU:HD23	4:D:156:LEU:O	1.87	0.74
13:M:36:THR:CG2	13:M:38:ILE:HD11	2.17	0.74
14:N:43:LEU:C	14:N:43:LEU:HD12	2.07	0.74
16:P:67:THR:HG22	16:P:69:THR:H	1.51	0.74
13:M:15:ASP:HB3	13:M:40:PRO:HB3	1.68	0.74
13:M:8:ILE:N	13:M:8:ILE:HD12	2.01	0.74
1:A:1163:C:H2'	1:A:1164:G:H8	1.53	0.74
11:K:4:VAL:HG21	11:K:30:ILE:CD1	2.17	0.74
1:A:116:A:H5'	1:A:116:A:H8	1.51	0.74
2:B:63:LEU:HD12	2:B:149:LEU:HD22	1.69	0.74
18:R:71:VAL:O	18:R:72:ARG:HD3	1.88	0.74
11:K:38:ILE:HD12	11:K:53:LEU:HB3	1.69	0.74
1:A:255:G:H1'	17:Q:15:GLN:NE2	2.03	0.73
3:C:111:SER:HB3	3:C:114:LEU:HD12	1.70	0.73
1:A:1189:C:P	10:J:49:ARG:HH22	2.10	0.73
1:A:958:A:H5'	1:A:959:A:OP2	1.88	0.73
3:C:78:ARG:HE	3:C:81:GLU:CB	2.00	0.73
16:P:81:ARG:HG2	16:P:83:GLU:HG2	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:37:ARG:HH11	3:C:37:ARG:HG3	1.53	0.73
1:A:1141:C:O2'	1:A:1142:G:H5'	1.88	0.73
11:K:3:GLN:HA	11:K:65:TYR:O	1.87	0.73
12:L:67:PRO:O	12:L:98:ARG:HD2	1.88	0.73
19:S:43:MET:HA	19:S:46:HIS:HD2	1.52	0.73
3:C:100:LEU:HD23	3:C:101:ASN:N	2.04	0.73
9:I:46:LEU:HB2	9:I:50:ARG:HH21	1.53	0.73
12:L:51:VAL:CG1	12:L:63:THR:HG22	2.18	0.73
1:A:189(I):G:O2'	1:A:189(J):G:H5'	1.88	0.73
1:A:49:U:C3'	1:A:50:A:H5"	2.19	0.73
2:B:194:ILE:HG22	2:B:195:ILE:N	2.04	0.73
11:K:81:ARG:HD3	18:R:73:LYS:HZ3	1.54	0.73
12:L:71:HIS:CD2	12:L:73:LEU:H	2.05	0.73
1:A:1282:C:H6	1:A:1282:C:H5'	1.52	0.73
5:E:140:THR:O	5:E:144:VAL:HG23	1.89	0.73
5:E:146:ARG:HH11	5:E:146:ARG:CB	2.02	0.72
10:J:6:LEU:HD12	10:J:18:ALA:HB2	1.70	0.72
1:A:1126:U:H2'	1:A:1126:U:O2	1.87	0.72
9:I:96:LYS:HB3	9:I:97:PRO:HD3	1.70	0.72
1:A:1477:C:H2'	1:A:1478:C:C6	2.25	0.72
3:C:25:LYS:H	3:C:25:LYS:CD	1.91	0.72
3:C:59:ALA:HB3	3:C:62:ASN:HD22	1.55	0.72
21:V:5:ARG:HE	21:V:14:ARG:HH22	1.37	0.72
1:A:1161:C:H2'	1:A:1162:C:C6	2.25	0.72
4:D:35:ARG:HA	4:D:37:TYR:CE1	2.25	0.72
10:J:47:VAL:O	10:J:58:ARG:HA	1.88	0.72
12:L:87:LYS:HA	12:L:87:LYS:HE3	1.70	0.72
15:O:61:GLN:HE22	15:O:64:ARG:NH2	1.88	0.72
18:R:21:ASN:O	18:R:25:LEU:HG	1.88	0.72
1:A:1230:C:H1'	13:M:125:LYS:HA	1.71	0.72
12:L:37:ARG:HG2	12:L:38:THR:N	2.03	0.72
4:D:208:ARG:HH11	4:D:208:ARG:HB3	1.55	0.72
7:G:17:TYR:CD2	7:G:58:LEU:HB2	2.25	0.72
19:S:15:LEU:O	19:S:18:VAL:HG12	1.90	0.72
19:S:18:VAL:O	19:S:22:ASN:HB2	1.89	0.72
13:M:3:ILE:HG23	13:M:56:ARG:HA	1.70	0.72
21:V:5:ARG:HE	21:V:14:ARG:NH1	1.88	0.72
1:A:1125:U:H2'	1:A:1125:U:O2	1.88	0.72
1:A:620:C:N1	4:D:134:LEU:HD13	2.05	0.72
18:R:21:ASN:HD22	18:R:21:ASN:C	1.91	0.72
19:S:50:VAL:O	19:S:57:VAL:HG22	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:78:ARG:HD2	3:C:78:ARG:O	1.89	0.71
3:C:78:ARG:HE	3:C:81:GLU:HG2	1.55	0.71
9:I:46:LEU:HB2	9:I:50:ARG:NH2	2.05	0.71
15:O:69:LEU:HD12	15:O:77:TYR:HB2	1.70	0.71
15:O:86:ILE:HG22	15:O:87:ARG:N	2.05	0.71
4:D:34:ARG:O	4:D:35:ARG:HB2	1.89	0.71
6:F:15:ASP:H	6:F:18:GLN:NE2	1.88	0.71
13:M:95:LEU:HB3	13:M:96:PRO:HD2	1.73	0.71
1:A:275:G:H5"	17:Q:13:LYS:HB3	1.70	0.71
3:C:33:LEU:HD13	14:N:24:VAL:HG21	1.71	0.71
4:D:17:LYS:HD2	4:D:19:TYR:HE1	1.54	0.71
4:D:28:PRO:O	4:D:29:LYS:HG3	1.91	0.71
15:O:16:ARG:HG3	15:O:16:ARG:HH11	1.55	0.71
2:B:181:LEU:HD23	2:B:195:ILE:O	1.91	0.71
1:A:235:C:H5'	17:Q:69:ARG:HG2	1.73	0.71
7:G:84:TYR:HD2	7:G:153:TYR:HE2	1.37	0.71
7:G:44:ASP:O	7:G:48:ILE:HG13	1.91	0.71
2:B:172:ARG:HH22	8:H:74:PRO:HB3	1.55	0.71
2:B:91:TRP:CH2	2:B:167:ALA:HA	2.26	0.71
12:L:122:LYS:HZ2	12:L:122:LYS:N	1.89	0.71
1:A:1208:C:H2'	1:A:1209:C:C6	2.26	0.71
12:L:79:VAL:HG21	12:L:96:ILE:CG2	2.19	0.71
21:V:5:ARG:NE	21:V:14:ARG:HH12	1.88	0.71
1:A:1405:G:O2'	1:A:1406:U:H5'	1.89	0.70
1:A:743:U:H2'	1:A:744:C:C6	2.26	0.70
2:B:94:GLY:O	2:B:102:ILE:HG13	1.91	0.70
3:C:107:ASN:ND2	3:C:110:LEU:HG	2.06	0.70
10:J:32:VAL:HA	10:J:72:ILE:HG22	1.72	0.70
11:K:44:ARG:HB3	11:K:44:ARG:NH1	2.06	0.70
5:E:68:GLN:O	5:E:69:ASN:HB3	1.91	0.70
10:J:76:ASN:HB2	10:J:79:THR:HG23	1.73	0.70
1:A:1427:U:H3	1:A:1473:A:H61	1.39	0.70
1:A:491:G:O2'	1:A:492:G:H5'	1.91	0.70
3:C:130:ARG:HG2	3:C:134:LYS:HE2	1.74	0.70
3:C:129:VAL:O	3:C:133:ILE:HG12	1.91	0.70
1:A:361:G:H2'	1:A:362:G:C5'	2.14	0.70
1:A:1263:C:H2'	1:A:1264:C:H6	1.57	0.70
11:K:96:LYS:CE	11:K:96:LYS:HA	2.18	0.70
20:T:50:ARG:HE	20:T:93:ILE:HG21	1.55	0.70
1:A:718:G:H5'	11:K:107:ASN:ND2	2.07	0.70
1:A:343:U:H2'	1:A:345:C:N4	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:53:THR:HG22	7:G:55:GLN:N	1.97	0.69
6:F:7:ASN:HB2	6:F:89:MET:HB3	1.73	0.69
1:A:1064:G:H4'	1:A:1065:U:OP1	1.91	0.69
1:A:279:A:C8	1:A:279:A:H5'	2.27	0.69
3:C:63:VAL:HG12	3:C:65:VAL:HG23	1.74	0.69
8:H:60:ARG:HG3	8:H:60:ARG:HH11	1.57	0.69
1:A:1369:C:H2'	1:A:1370:G:C8	2.27	0.69
2:B:92:LEU:HD23	2:B:92:LEU:N	2.07	0.69
1:A:1277:C:HO2'	1:A:1279:A:H8	1.41	0.69
13:M:7:GLU:OE2	13:M:21:ILE:HA	1.92	0.69
2:B:50:ARG:NH1	2:B:50:ARG:HB2	2.07	0.69
10:J:59:GLU:OE1	14:N:44:ARG:NH1	2.21	0.69
1:A:1314:C:H5"	19:S:5:LYS:NZ	2.07	0.69
4:D:61:GLN:HA	4:D:61:GLN:HE21	1.56	0.69
2:B:71:ALA:CB	2:B:205:ILE:HD13	2.22	0.69
14:N:22:ARG:NH1	14:N:29:ALA:HB2	2.07	0.69
17:Q:39:LYS:HD2	17:Q:41:TYR:CZ	2.28	0.69
1:A:601:C:O2'	1:A:602:A:H5'	1.92	0.69
2:B:78:GLU:OE1	2:B:210:SER:HA	1.92	0.69
3:C:13:ILE:O	3:C:15:ARG:N	2.25	0.69
4:D:69:ILE:HD11	4:D:99:ARG:NE	2.08	0.69
5:E:72:ILE:HG23	5:E:138:LEU:HD13	1.73	0.69
8:H:64:LYS:HG2	8:H:79:VAL:HG21	1.73	0.69
2:B:95:MET:HA	2:B:102:ILE:HG21	1.75	0.69
12:L:29:ARG:HD3	12:L:58:SER:HB3	1.75	0.69
13:M:80:LEU:H	13:M:80:LEU:HD23	1.57	0.69
3:C:99:ALA:O	3:C:100:LEU:HB2	1.92	0.69
14:N:56:ARG:CG	14:N:57:LYS:H	2.05	0.69
20:T:41:LYS:NZ	20:T:41:LYS:HB2	2.08	0.69
1:A:702:A:H4'	1:A:703:G:OP2	1.92	0.68
1:A:858:G:H5"	1:A:858:G:H8	1.59	0.68
18:R:23:GLU:CD	18:R:23:GLU:H	1.97	0.68
1:A:386:C:H2'	1:A:387:U:H5'	1.75	0.68
3:C:7:ILE:HG23	3:C:15:ARG:HG2	1.75	0.68
6:F:26:ILE:O	6:F:30:LEU:HG	1.93	0.68
17:Q:103:LYS:HB3	17:Q:103:LYS:NZ	2.08	0.68
1:A:1045:C:H2'	1:A:1046:A:C5'	2.23	0.68
1:A:1228:C:H4'	13:M:115:THR:HA	1.75	0.68
1:A:954:G:H2'	1:A:955:U:C6	2.28	0.68
6:F:2:ARG:NE	6:F:69:GLU:HG2	2.07	0.68
3:C:12:GLY:HA3	14:N:56:ARG:CZ	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:4:TYR:O	9:I:83:ALA:HA	1.92	0.68
10:J:78:LYS:HD2	10:J:81:GLU:OE1	1.93	0.68
1:A:718:G:C5'	11:K:107:ASN:HD22	2.06	0.68
1:A:1251:A:H4'	9:I:11:GLU:OE2	1.93	0.68
13:M:22:TYR:O	13:M:24:ILE:N	2.26	0.68
13:M:2:ARG:HA	13:M:7:GLU:O	1.94	0.68
1:A:1060:C:O2'	1:A:1061:G:H5'	1.93	0.68
12:L:85:ARG:HE	12:L:93:ARG:HB3	1.59	0.68
20:T:22:LYS:O	20:T:26:ILE:HG13	1.94	0.68
5:E:78:VAL:HG11	5:E:130:ALA:O	1.94	0.68
11:K:4:VAL:HG21	11:K:30:ILE:HD11	1.75	0.68
12:L:122:LYS:H	12:L:122:LYS:HZ2	1.39	0.68
12:L:24:LYS:O	12:L:26:ALA:N	2.27	0.68
19:S:64:ASN:HD22	19:S:65:MET:H	1.40	0.68
1:A:1366:C:H2'	1:A:1367:C:H6	1.58	0.68
2:B:136:LEU:HD13	2:B:136:LEU:O	1.93	0.68
1:A:1241:G:H2'	1:A:1242:C:C6	2.28	0.68
1:A:386:C:O2'	1:A:387:U:H5'	1.94	0.68
9:I:117:LYS:O	9:I:118:ALA:HB3	1.94	0.68
14:N:44:ARG:HH11	14:N:44:ARG:HG3	1.58	0.68
17:Q:39:LYS:HD2	17:Q:41:TYR:CE1	2.29	0.68
1:A:457:C:H2'	1:A:458:C:H6	1.59	0.67
16:P:59:TRP:HA	16:P:62:VAL:HG23	1.76	0.67
2:B:175:PHE:CD2	8:H:70:GLN:HB3	2.29	0.67
4:D:35:ARG:H	4:D:36:PRO:HD3	1.59	0.67
5:E:123:ASN:ND2	5:E:124:PRO:HD2	2.09	0.67
3:C:155:ARG:HH21	3:C:160:GLU:HA	1.59	0.67
1:A:835:U:OP1	18:R:49:ARG:NH2	2.27	0.67
1:A:1363(A):A:H1'	1:A:1365:G:N7	2.09	0.67
2:B:112:LEU:HB3	2:B:136:LEU:HD23	1.77	0.67
5:E:48:PRO:O	5:E:52:GLN:HG2	1.94	0.67
4:D:88:THR:O	4:D:88:THR:HG22	1.94	0.67
12:L:51:VAL:CG1	12:L:52:ALA:H	2.08	0.67
19:S:48:ILE:N	19:S:48:ILE:HD12	2.09	0.67
1:A:1027:C:H6	1:A:1027:C:H5'	1.60	0.67
3:C:126:ARG:HH11	3:C:126:ARG:HG2	1.59	0.67
12:L:122:LYS:N	12:L:122:LYS:NZ	2.41	0.67
1:A:203:U:H5"	1:A:204:U:OP1	1.94	0.67
1:A:262:A:H5'	20:T:67:LYS:HG2	1.77	0.67
1:A:302:G:H5"	12:L:13:LYS:HZ1	1.58	0.67
2:B:134:HIS:HA	2:B:137:GLU:HG2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:35:ARG:H	4:D:36:PRO:CD	2.07	0.67
10:J:30:ALA:C	10:J:32:VAL:H	1.96	0.67
1:A:152:A:H5'	1:A:153:C:OP2	1.95	0.67
3:C:81:GLU:O	3:C:85:VAL:HG23	1.95	0.67
4:D:60:LYS:HD2	4:D:206:TYR:OH	1.95	0.67
6:F:100:ASN:HD22	18:R:8:LYS:CG	2.07	0.66
21:V:5:ARG:HE	21:V:14:ARG:NH2	1.93	0.66
12:L:37:ARG:HH22	12:L:53:LYS:HZ3	1.41	0.66
13:M:33:LEU:HD13	13:M:40:PRO:HA	1.77	0.66
1:A:21:G:H2'	1:A:22:G:C8	2.30	0.66
3:C:178:ARG:HH11	3:C:206:VAL:HG22	1.59	0.66
14:N:49:LYS:HB2	14:N:51:GLN:HG3	1.78	0.66
1:A:664:G:H22	1:A:741:G:H1	1.42	0.66
1:A:1189:C:OP1	10:J:49:ARG:NH2	2.26	0.66
2:B:215:LEU:HD13	2:B:215:LEU:O	1.95	0.66
8:H:127:LEU:HD23	8:H:127:LEU:H	1.60	0.66
4:D:146:ALA:HA	4:D:181:LYS:HA	1.77	0.66
19:S:79:TYR:CE2	19:S:80:ARG:HB2	2.30	0.66
1:A:639:G:O2'	1:A:640:A:H5'	1.96	0.66
14:N:23:CYS:HB2	14:N:39:CYS:HB3	1.76	0.66
1:A:489:C:H2'	1:A:490:G:C8	2.29	0.66
1:A:522:C:H41	12:L:49:ARG:NH2	1.88	0.66
3:C:133:ILE:HG22	3:C:167:ALA:HB3	1.78	0.66
9:I:9:ARG:HD3	9:I:104:ASP:HB3	1.76	0.66
12:L:32:VAL:HG22	12:L:78:VAL:HG22	1.76	0.66
19:S:44:VAL:HA	19:S:61:ILE:HD12	1.78	0.66
1:A:1169:A:H2'	1:A:1170:A:C8	2.31	0.66
2:B:172:ARG:HH11	2:B:172:ARG:HG3	1.61	0.66
6:F:101:ALA:HB1	18:R:13:GLU:HG3	1.78	0.66
11:K:40:TYR:HB3	11:K:44:ARG:HB2	1.75	0.66
16:P:59:TRP:HB3	16:P:64:ALA:HB2	1.76	0.66
1:A:975:A:H5"	1:A:976:G:O5'	1.96	0.65
10:J:6:LEU:CD2	10:J:94:ILE:HG12	2.26	0.65
15:O:63:ARG:HH11	15:O:63:ARG:HG3	1.61	0.65
2:B:63:LEU:HD23	2:B:64:PHE:N	2.12	0.65
2:B:17:ARG:NH1	2:B:18:TRP:HA	2.11	0.65
2:B:175:PHE:HD2	8:H:70:GLN:HB3	1.61	0.65
12:L:20:VAL:HG12	12:L:20:VAL:O	1.97	0.65
1:A:1130:A:H2'	1:A:1130:A:N3	2.12	0.65
1:A:1491:G:C6	26:A:2800:RPO:H2	2.31	0.65
1:A:820:U:H4'	1:A:821:G:OP2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:954:G:H2'	1:A:955:U:H6	1.62	0.65
1:A:957:U:C3'	1:A:958:A:H5"	2.27	0.65
4:D:69:ILE:HD11	4:D:99:ARG:CZ	2.26	0.65
1:A:1399:C:H4'	1:A:1400:C:C5'	2.23	0.65
8:H:65:TYR:HA	8:H:79:VAL:HG23	1.79	0.65
21:V:12:ILE:HD13	21:V:21:ARG:NE	2.12	0.65
4:D:148:ALA:HB3	4:D:151:SER:HB2	1.79	0.65
1:A:1244:C:HO2'	1:A:1245:A:H8	1.43	0.65
3:C:173:PRO:HB2	3:C:176:THR:CG2	2.26	0.65
1:A:159:G:H21	1:A:161:A:H3'	1.62	0.65
13:M:104:THR:HG22	13:M:105:ASN:H	1.61	0.65
1:A:1218:C:H2'	1:A:1219:U:C6	2.32	0.65
2:B:10:HIS:HB3	2:B:204:SER:HB2	1.79	0.65
5:E:85:ILE:HG13	5:E:131:THR:HG22	1.78	0.65
3:C:189:ARG:HB3	3:C:189:ARG:HH11	1.61	0.64
6:F:46:ARG:O	6:F:57:GLN:HB2	1.97	0.64
12:L:71:HIS:HA	12:L:98:ARG:NH2	2.10	0.64
1:A:1323:G:H2'	1:A:1324:A:C8	2.33	0.64
1:A:180:U:C2'	1:A:181:G:H5'	2.26	0.64
1:A:390:C:H2'	1:A:391:G:C8	2.32	0.64
8:H:63:LEU:H	8:H:63:LEU:HD22	1.61	0.64
2:B:10:HIS:CG	2:B:11:PHE:H	2.14	0.64
3:C:78:ARG:HE	3:C:81:GLU:CG	2.09	0.64
6:F:101:ALA:CB	18:R:13:GLU:HG3	2.27	0.64
8:H:86:ILE:CG2	8:H:133:LEU:HD23	2.20	0.64
1:A:797:C:O2'	1:A:798:G:H5'	1.96	0.64
1:A:957:U:H2'	1:A:958:A:H5"	1.79	0.64
10:J:20:LYS:NZ	10:J:88:LEU:H	1.95	0.64
10:J:60:HIS:HB3	14:N:58:ALA:HB3	1.78	0.64
12:L:37:ARG:HB3	12:L:37:ARG:NH1	2.12	0.64
8:H:9:MET:SD	8:H:32:LYS:HG2	2.37	0.64
9:I:46:LEU:C	9:I:48:PRO:HD2	2.17	0.64
10:J:4:ILE:HG23	10:J:96:ILE:HG23	1.79	0.64
3:C:36:GLN:NE2	14:N:46:LEU:HD13	2.12	0.64
1:A:1306:A:O2'	13:M:108:THR:HG21	1.98	0.64
1:A:159:G:H5"	1:A:159:G:H8	1.63	0.64
1:A:824:C:H2'	1:A:825:G:H8	1.63	0.64
1:A:865:A:H5'	1:A:1078:U:O4	1.97	0.64
3:C:190:THR:HG21	3:C:192:TYR:CZ	2.33	0.64
5:E:5:LYS:HB2	5:E:108:LEU:HD11	1.79	0.64
12:L:83:GLY:HA2	12:L:94:TYR:CA	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:72:ARG:O	18:R:73:LYS:HB3	1.97	0.64
1:A:1007:C:H2'	1:A:1008:C:C6	2.32	0.64
1:A:1352:C:H2'	1:A:1353:G:C8	2.33	0.64
4:D:2:ARG:HD2	4:D:117:ARG:CZ	2.27	0.64
1:A:52:G:O2'	1:A:53:A:H5'	1.98	0.64
2:B:50:ARG:HH11	2:B:50:ARG:CB	2.10	0.64
4:D:154:LEU:HD23	4:D:155:GLU:H	1.62	0.64
5:E:145:GLU:O	5:E:149:LYS:HG3	1.98	0.64
17:Q:51:LYS:O	17:Q:54:ASP:HB2	1.98	0.64
1:A:166:G:O2'	1:A:167:G:H5'	1.98	0.64
1:A:556:C:O2'	1:A:557:G:H5'	1.98	0.64
1:A:743:U:H2'	1:A:744:C:H6	1.61	0.64
10:J:29:GLY:HA2	10:J:76:ASN:HD21	1.60	0.64
1:A:718:G:C5'	11:K:107:ASN:ND2	2.60	0.64
16:P:43:LYS:HB3	16:P:48:TRP:CD1	2.32	0.64
13:M:76:ASN:O	13:M:80:LEU:HD23	1.99	0.63
4:D:6:PRO:HB2	4:D:9:ARG:HD2	1.79	0.63
10:J:44:ARG:HG2	10:J:44:ARG:HH11	1.64	0.63
13:M:64:LYS:NZ	13:M:68:GLU:HG2	2.13	0.63
7:G:45:ALA:O	7:G:49:ILE:HG13	1.98	0.63
10:J:49:ARG:HG2	10:J:58:ARG:O	1.99	0.63
1:A:1346:A:N1	1:A:1374:A:H5"	2.13	0.63
2:B:181:LEU:HA	2:B:195:ILE:HB	1.79	0.63
3:C:133:ILE:CG2	3:C:167:ALA:HB3	2.28	0.63
4:D:11:CYS:HA	4:D:18:LEU:HD12	1.80	0.63
5:E:8:LEU:CD1	5:E:27:LEU:HB2	2.28	0.63
7:G:148:ARG:HD2	11:K:49:TYR:CE1	2.33	0.63
13:M:35:LYS:NZ	13:M:35:LYS:HB3	2.13	0.63
1:A:1423:G:H2'	1:A:1424:C:C6	2.33	0.63
1:A:190:U:O2	20:T:98:SER:HB2	1.97	0.63
11:K:115:PHE:O	11:K:116:ARG:HB3	1.98	0.63
17:Q:100:ARG:HE	17:Q:100:ARG:HA	1.64	0.63
17:Q:100:ARG:NE	17:Q:100:ARG:HA	2.14	0.63
6:F:94:GLN:HE21	18:R:17:ARG:HE	1.47	0.63
3:C:57:GLU:HB2	3:C:64:ALA:HB2	1.80	0.63
1:A:720:C:H3'	1:A:721:G:H5"	1.80	0.63
1:A:731:G:OP1	1:A:766:A:H1'	1.98	0.63
1:A:953:G:H5'	1:A:965:A:H61	1.64	0.63
4:D:24:ARG:C	4:D:26:TYR:H	2.01	0.63
19:S:32:THR:HG22	19:S:33:TRP:H	1.64	0.63
20:T:60:ALA:O	20:T:66:HIS:ND1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:81:ARG:NH1	18:R:73:LYS:HE2	2.14	0.63
19:S:19:LEU:HD12	19:S:20:GLU:N	2.13	0.63
2:B:13:HIS:O	2:B:14:GLU:O	2.16	0.63
7:G:135:LYS:HE3	7:G:139:ASP:OD1	1.99	0.63
7:G:93:ARG:HG3	7:G:93:ARG:HH11	1.64	0.63
8:H:118:VAL:C	8:H:119:LEU:HD23	2.18	0.63
1:A:1250:A:H4'	9:I:67:GLY:O	1.98	0.63
11:K:100:ASP:HB2	18:R:73:LYS:HD2	1.79	0.63
17:Q:44:HIS:CD2	17:Q:46:PRO:HG3	2.34	0.63
18:R:29:LEU:HD11	18:R:64:LEU:HD13	1.81	0.63
1:A:437:U:C2'	1:A:438:G:H5'	2.29	0.62
6:F:22:GLU:O	6:F:26:ILE:HG12	1.98	0.62
7:G:75:ARG:HD2	7:G:88:MET:SD	2.39	0.62
21:V:11:LYS:HB3	21:V:21:ARG:HD2	1.81	0.62
1:A:384:G:H2'	1:A:385:C:C6	2.33	0.62
1:A:627:G:O2'	1:A:628:G:H5'	2.00	0.62
4:D:29:LYS:C	4:D:31:ALA:H	2.01	0.62
16:P:67:THR:HG22	16:P:69:THR:N	2.14	0.62
19:S:62:THR:HG22	19:S:63:GLU:N	2.13	0.62
1:A:1019:C:C2'	1:A:1020:U:H5'	2.29	0.62
1:A:1132:C:H2'	1:A:1133:G:H8	1.63	0.62
1:A:477:A:O2'	1:A:479:C:H5'	2.00	0.62
1:A:56:U:H2'	1:A:57:G:C8	2.35	0.62
3:C:32:LEU:HD21	14:N:52:LEU:HD23	1.81	0.62
3:C:21:TRP:HB3	3:C:58:ARG:HB2	1.81	0.62
9:I:111:LYS:HG3	9:I:117:LYS:HA	1.82	0.62
9:I:96:LYS:O	9:I:99:GLY:N	2.28	0.62
2:B:133:LYS:O	2:B:137:GLU:HG2	1.99	0.62
1:A:522:C:N4	12:L:49:ARG:HH22	1.89	0.62
18:R:10:THR:O	18:R:11:LEU:HB2	1.98	0.62
1:A:443:C:H2'	1:A:444:C:H6	1.64	0.62
1:A:877:C:H5"	8:H:88:LYS:HD3	1.80	0.62
2:B:205:ILE:O	2:B:209:LEU:HB2	1.99	0.62
4:D:161:LEU:HD13	4:D:180:MET:CG	2.30	0.62
1:A:1020:U:C3'	1:A:1021:G:H5"	2.29	0.62
1:A:1208:C:H2'	1:A:1209:C:H6	1.63	0.62
1:A:1353:G:H2'	1:A:1354:C:C6	2.35	0.62
1:A:750:G:N3	15:O:22:GLY:HA3	2.15	0.62
2:B:112:LEU:HD11	2:B:135:GLU:OE1	1.99	0.62
13:M:77:ILE:HA	13:M:80:LEU:HD21	1.80	0.62
1:A:1054:C:H4'	1:A:1055:A:H5'	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1140:C:H2'	1:A:1141:C:H5"	1.82	0.62
1:A:1166:G:C3'	1:A:1168:A:H5"	2.28	0.62
1:A:542:G:O2'	1:A:543:C:H5'	1.99	0.62
1:A:302:G:H5"	12:L:13:LYS:NZ	2.15	0.62
10:J:47:VAL:HG22	14:N:40:ARG:HB2	1.81	0.62
1:A:17:U:H2'	1:A:18:C:C6	2.34	0.62
2:B:217:ILE:C	2:B:219:ALA:H	2.02	0.62
7:G:64:ALA:O	7:G:68:VAL:HG23	2.00	0.62
13:M:7:GLU:HG3	13:M:21:ILE:HG23	1.82	0.62
14:N:2:ARG:O	14:N:4:ALA:N	2.32	0.62
17:Q:39:LYS:HG2	17:Q:40:LYS:N	2.15	0.62
20:T:41:LYS:HB2	20:T:41:LYS:HZ3	1.63	0.62
20:T:89:GLY:O	20:T:90:ALA:HB3	2.00	0.62
1:A:1427:U:H2'	1:A:1428:A:C8	2.35	0.62
1:A:839:U:H3'	1:A:840:C:C5'	2.25	0.62
2:B:6:GLU:HG3	2:B:207:LEU:HD11	1.82	0.62
3:C:37:ARG:HG3	3:C:37:ARG:NH1	2.11	0.62
19:S:61:ILE:HD13	19:S:61:ILE:C	2.20	0.62
20:T:3:LEU:O	20:T:5:ALA:N	2.32	0.62
1:A:166:G:H2'	1:A:167:G:H8	1.65	0.61
1:A:673:G:H2'	1:A:674:G:C8	2.35	0.61
2:B:233:VAL:O	2:B:233:VAL:HG12	2.00	0.61
7:G:138:GLU:O	7:G:142:ARG:HG3	2.00	0.61
10:J:73:ILE:O	10:J:74:ASN:HB2	2.00	0.61
13:M:34:GLU:C	13:M:36:THR:H	2.02	0.61
20:T:50:ARG:NH1	20:T:50:ARG:HG2	2.14	0.61
1:A:1026:G:H2'	1:A:1027:C:H5"	1.81	0.61
2:B:11:PHE:CD1	2:B:35:ILE:HG23	2.35	0.61
4:D:149:GLU:HA	4:D:152:ARG:NH2	2.14	0.61
10:J:1:LYS:N	10:J:75:PRO:HD3	2.14	0.61
1:A:384:G:H2'	1:A:385:C:H6	1.66	0.61
1:A:412:A:H61	4:D:34:ARG:HB3	1.65	0.61
17:Q:79:GLY:O	17:Q:81:MET:HG2	1.99	0.61
18:R:28:PHE:HA	18:R:36:LEU:HD12	1.82	0.61
18:R:39:ARG:NH2	18:R:40:ARG:HG3	2.15	0.61
19:S:32:THR:HG22	19:S:33:TRP:N	2.14	0.61
21:V:5:ARG:NE	21:V:14:ARG:HH22	1.97	0.61
1:A:1001(A):G:H2'	1:A:1002:G:O4'	2.00	0.61
19:S:27:LYS:CG	19:S:28:ARG:H	2.12	0.61
19:S:61:ILE:HD13	19:S:62:THR:N	2.14	0.61
1:A:307:C:H5'	1:A:308:C:OP2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:43:LEU:N	6:F:43:LEU:HD22	2.15	0.61
16:P:18:ARG:O	16:P:20:VAL:HG13	2.01	0.61
1:A:1302:U:C5	13:M:16:VAL:HG21	2.35	0.61
13:M:22:TYR:HB2	13:M:66:GLU:OE2	2.00	0.61
19:S:4:LEU:O	19:S:5:LYS:CB	2.48	0.61
20:T:86:GLU:HA	20:T:86:GLU:OE1	2.00	0.61
1:A:1342:C:O2'	1:A:1343:G:H5'	2.00	0.61
2:B:27:TYR:HB3	2:B:35:ILE:O	2.00	0.61
3:C:14:THR:O	3:C:15:ARG:HB2	2.00	0.61
4:D:10:LEU:O	4:D:14:GLU:HG2	2.01	0.61
17:Q:26:PHE:CZ	17:Q:35:ILE:HD11	2.36	0.61
1:A:1263:C:H2'	1:A:1264:C:C6	2.35	0.61
1:A:1347:G:N2	1:A:1373:G:H2'	2.15	0.61
1:A:251:G:C2'	1:A:252:U:H5"	2.28	0.61
3:C:174:LEU:HD21	3:C:200:TYR:CE2	2.36	0.61
10:J:80:ILE:O	10:J:84:MET:HB2	2.01	0.61
1:A:957:U:C2'	1:A:958:A:H5"	2.30	0.61
9:I:124:TYR:HD2	9:I:127:ARG:HG2	1.64	0.61
9:I:92:ARG:HG3	9:I:92:ARG:HH11	1.66	0.61
1:A:345:C:H4'	1:A:346:G:O5'	2.01	0.60
3:C:27:GLN:HA	3:C:30:HIS:CD2	2.22	0.60
8:H:4:ASP:CG	8:H:85:ARG:HH11	2.04	0.60
20:T:43:GLU:O	20:T:93:ILE:HG13	2.01	0.60
2:B:109:LEU:HD22	2:B:147:ARG:NH2	2.16	0.60
8:H:119:LEU:HD12	8:H:124:ALA:HA	1.83	0.60
10:J:15:ASP:O	10:J:19:GLN:HB2	2.01	0.60
15:O:23:SER:OG	15:O:26:VAL:HG23	2.01	0.60
20:T:67:LYS:NZ	20:T:67:LYS:HB2	2.16	0.60
21:V:4:ASP:O	21:V:10:GLY:HA3	2.00	0.60
2:B:79:ALA:HB3	2:B:86:TYR:HD2	1.65	0.60
9:I:91:TYR:C	9:I:93:ALA:H	2.04	0.60
1:A:1030(C):G:H2'	1:A:1030(D):A:C8	2.36	0.60
1:A:1135:U:H4'	1:A:1136:U:OP1	2.01	0.60
1:A:131:C:H2'	1:A:132:C:C6	2.37	0.60
1:A:390:C:O3'	16:P:28:ARG:NH2	2.34	0.60
3:C:118:ARG:NH1	3:C:139:ARG:HH12	1.99	0.60
9:I:41:ARG:HH11	9:I:41:ARG:HG2	1.65	0.60
10:J:3:ARG:HA	10:J:71:ASP:OD1	2.02	0.60
9:I:126:LYS:HB3	13:M:125:LYS:NZ	2.16	0.60
4:D:17:LYS:HD2	4:D:19:TYR:CE1	2.36	0.60
6:F:47:ARG:HE	6:F:47:ARG:H	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:61:ASN:O	13:M:62:THR:CB	2.49	0.60
18:R:21:ASN:HD21	18:R:23:GLU:HG2	1.67	0.60
1:A:1330:U:C2'	1:A:1331:G:H5'	2.30	0.60
13:M:49:GLU:OE1	13:M:49:GLU:HA	2.02	0.60
18:R:21:ASN:ND2	18:R:23:GLU:HG2	2.16	0.60
19:S:41:PRO:O	19:S:44:VAL:HG23	2.02	0.60
1:A:530:G:O6	22:W:3:C:H1'	2.02	0.60
1:A:67:C:O2'	1:A:171:A:H1'	2.01	0.60
1:A:344:A:H5"	1:A:345:C:H5	1.67	0.60
5:E:146:ARG:HH11	5:E:146:ARG:HB3	1.66	0.60
10:J:55:LYS:O	10:J:58:ARG:NH1	2.35	0.60
12:L:23:LEU:C	12:L:25:GLY:H	2.03	0.60
12:L:2:THR:OG1	12:L:5:GLN:HG3	2.02	0.60
14:N:28:ARG:HG2	14:N:28:ARG:HH11	1.67	0.60
14:N:1:ALA:HB1	14:N:6:ILE:HD11	1.82	0.60
20:T:46:LEU:HD12	20:T:93:ILE:HB	1.84	0.60
1:A:1045:C:C2'	1:A:1046:A:H5"	2.29	0.60
1:A:1048:G:H8	1:A:1048:G:H5'	1.65	0.60
1:A:858:G:C8	1:A:858:G:C5'	2.82	0.60
2:B:109:LEU:HD21	2:B:140:GLN:HE22	1.65	0.60
9:I:27:VAL:HA	9:I:62:ILE:O	2.00	0.60
9:I:2:GLN:HB3	9:I:19:ARG:HG2	1.83	0.60
9:I:45:ALA:HB1	9:I:76:ILE:CG2	2.31	0.60
13:M:16:VAL:O	13:M:19:THR:HB	2.02	0.60
19:S:15:LEU:O	19:S:19:LEU:HG	2.01	0.60
1:A:1305:G:P	21:V:1:GLY:N	2.75	0.60
1:A:501:C:O2'	1:A:502:G:H5'	2.02	0.60
1:A:818:G:C3'	1:A:819:A:H5"	2.31	0.60
2:B:133:LYS:HG2	2:B:137:GLU:OE2	2.02	0.60
3:C:87:ARG:HA	3:C:90:LEU:HG	1.84	0.60
7:G:14:ASP:OD1	7:G:43:TYR:OH	2.19	0.60
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.84	0.60
11:K:77:THR:HG22	11:K:77:THR:O	2.02	0.60
14:N:22:ARG:O	14:N:23:CYS:C	2.39	0.60
10:J:61:PHE:CE1	14:N:57:LYS:HG2	2.36	0.60
1:A:1136:U:H5"	1:A:1137:C:OP2	2.01	0.60
1:A:1163:C:H2'	1:A:1164:G:C8	2.35	0.60
1:A:1330:U:OP1	13:M:22:TYR:O	2.20	0.60
1:A:35:G:H2'	1:A:36:C:C6	2.37	0.60
1:A:8:A:H5"	5:E:97:ILE:CG2	2.32	0.60
2:B:135:GLU:O	2:B:139:LEU:HG	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:5:GLY:HA3	9:I:82:ARG:HG3	1.84	0.60
10:J:37:PRO:O	10:J:38:LEU:HB2	2.01	0.60
10:J:80:ILE:HD12	10:J:80:ILE:H	1.66	0.60
11:K:105:PRO:C	11:K:107:ASN:H	2.04	0.60
1:A:445:G:H2'	1:A:446:G:H8	1.66	0.59
3:C:2:ASN:O	3:C:3:LYS:HG2	2.02	0.59
7:G:14:ASP:HB3	7:G:18:GLY:N	2.17	0.59
1:A:718:G:C4'	11:K:107:ASN:HD22	2.15	0.59
11:K:44:ARG:HB3	11:K:44:ARG:HH11	1.66	0.59
10:J:59:GLU:OE2	14:N:57:LYS:HE3	2.01	0.59
1:A:101:A:O2'	1:A:102:G:H5'	2.01	0.59
4:D:86:GLY:O	4:D:88:THR:N	2.35	0.59
7:G:107:ALA:HA	7:G:110:ARG:HD2	1.84	0.59
11:K:96:LYS:HE2	11:K:96:LYS:CA	2.21	0.59
15:O:15:ALA:HB1	15:O:20:ASP:HB3	1.82	0.59
17:Q:80:ARG:O	17:Q:80:ARG:HG3	2.01	0.59
1:A:460:G:H3'	1:A:461:A:H5"	1.80	0.59
1:A:501:C:H2'	1:A:502:G:H8	1.67	0.59
6:F:33:TYR:HE2	6:F:78:GLU:HG2	1.67	0.59
3:C:146:LYS:HE2	3:C:204:GLY:H	1.67	0.59
6:F:30:LEU:HB3	6:F:35:ALA:HB3	1.83	0.59
8:H:56:LYS:CD	8:H:56:LYS:H	2.16	0.59
10:J:48:ILE:N	10:J:48:ILE:HD12	2.18	0.59
15:O:2:ILE:HD12	15:O:2:ILE:N	2.16	0.59
1:A:192:U:H5'	20:T:95:GLY:HA2	1.84	0.59
3:C:100:LEU:HD23	3:C:100:LEU:C	2.23	0.59
3:C:206:VAL:HG12	3:C:207:ILE:N	2.17	0.59
13:M:25:GLY:O	13:M:27:ALA:N	2.35	0.59
16:P:52:ASP:OD2	16:P:55:ARG:HG3	2.03	0.59
18:R:32:THR:HA	18:R:68:GLU:HB2	1.84	0.59
20:T:58:LYS:O	20:T:61:LYS:HB2	2.03	0.59
1:A:997:U:C3'	1:A:998:G:H5"	2.33	0.59
3:C:187:LEU:O	3:C:188:ALA:HB2	2.02	0.59
3:C:69:VAL:HG12	3:C:70:ALA:N	2.17	0.59
7:G:14:ASP:HB3	7:G:18:GLY:H	1.67	0.59
1:A:1156:G:H2'	1:A:1157:A:H5"	1.85	0.59
1:A:976:G:H5"	1:A:1358:U:O2'	2.03	0.59
8:H:103:VAL:HG21	8:H:109:ILE:O	2.03	0.59
8:H:24:THR:CG2	8:H:63:LEU:HD21	2.33	0.59
10:J:28:SER:HB3	10:J:82:GLN:HE21	1.68	0.59
12:L:28:PHE:HB3	12:L:81:ILE:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:22:ARG:HH11	14:N:22:ARG:HG2	1.66	0.59
14:N:5:LEU:C	14:N:7:GLU:H	2.05	0.59
1:A:1148:U:H2'	1:A:1149:C:O4'	2.03	0.59
1:A:1176:A:H2'	1:A:1177:G:C8	2.38	0.59
1:A:677:U:H3	1:A:713:G:H22	1.49	0.59
1:A:994:A:N3	1:A:994:A:H2'	2.17	0.59
2:B:172:ARG:NH1	2:B:172:ARG:HG3	2.18	0.59
2:B:19:ASN:C	2:B:19:ASN:HD22	2.06	0.59
5:E:76:ILE:HG22	5:E:87:LEU:HB2	1.85	0.59
12:L:37:ARG:NH2	12:L:53:LYS:NZ	2.49	0.59
13:M:35:LYS:HZ3	13:M:35:LYS:HB3	1.68	0.59
13:M:64:LYS:HZ1	13:M:68:GLU:HG2	1.68	0.59
15:O:86:ILE:HG22	15:O:87:ARG:H	1.67	0.59
1:A:1144:G:N2	1:A:1146:A:H62	1.97	0.59
2:B:91:TRP:HZ3	2:B:166:ILE:HG22	1.68	0.59
2:B:16:LYS:HD2	2:B:29:GLU:OE2	2.02	0.59
3:C:82:ARG:C	3:C:84:ARG:H	2.06	0.59
5:E:84:LYS:HB3	5:E:119:LEU:HB2	1.83	0.59
10:J:74:ASN:O	10:J:76:ASN:N	2.31	0.59
20:T:1:ARG:O	20:T:2:ASN:HB2	2.02	0.59
1:A:1480:G:H4'	1:A:1481:U:OP2	2.02	0.59
1:A:636:U:O2'	1:A:637:G:H5'	2.03	0.59
2:B:136:LEU:HD13	2:B:140:GLN:OE1	2.02	0.59
2:B:49:PHE:O	2:B:52:ILE:HB	2.03	0.59
2:B:79:ALA:HB3	2:B:86:TYR:CD2	2.37	0.59
4:D:50:PRO:HB2	4:D:55:VAL:HG23	1.83	0.59
5:E:70:GLY:CA	5:E:112:THR:HG22	2.30	0.59
5:E:147:LEU:CD2	8:H:79:VAL:HG22	2.33	0.59
5:E:8:LEU:HD13	5:E:27:LEU:HB2	1.84	0.59
9:I:47:GLU:N	9:I:48:PRO:HD2	2.17	0.59
1:A:116:A:H2'	1:A:117:G:O4'	2.02	0.58
1:A:648:A:H8	1:A:648:A:H5'	1.68	0.58
2:B:94:GLY:C	2:B:102:ILE:HG13	2.24	0.58
2:B:22:PHE:CZ	2:B:183:ASP:HA	2.38	0.58
3:C:179:ALA:O	3:C:180:ASN:C	2.41	0.58
7:G:91:SER:HB2	7:G:92:PRO:HD2	1.85	0.58
10:J:25:ALA:CB	10:J:83:LEU:HD11	2.24	0.58
14:N:7:GLU:C	14:N:7:GLU:OE1	2.41	0.58
2:B:194:ILE:CG2	2:B:195:ILE:N	2.66	0.58
1:A:1262:C:H2'	1:A:1263:C:C6	2.38	0.58
1:A:841:U:H5"	1:A:848:C:C2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:87:VAL:O	4:D:89:GLY:N	2.32	0.58
5:E:72:ILE:HG23	5:E:138:LEU:CD1	2.34	0.58
7:G:77:ARG:HB2	7:G:155:TRP:CZ3	2.38	0.58
10:J:73:ILE:HG22	10:J:74:ASN:H	1.67	0.58
12:L:29:ARG:CD	12:L:58:SER:HB3	2.34	0.58
2:B:11:PHE:HD1	2:B:35:ILE:HG23	1.69	0.58
3:C:154:GLY:O	3:C:155:ARG:HB2	2.03	0.58
4:D:37:TYR:N	4:D:37:TYR:CD1	2.68	0.58
10:J:23:GLU:C	10:J:25:ALA:H	2.06	0.58
13:M:32:ALA:O	13:M:36:THR:HB	2.03	0.58
2:B:222:GLY:O	2:B:224:VAL:HG23	2.03	0.58
4:D:153:ASN:HA	4:D:158:ARG:NH2	2.18	0.58
4:D:37:TYR:CE2	4:D:44:GLN:HG2	2.38	0.58
8:H:6:ILE:O	8:H:10:LEU:HG	2.04	0.58
10:J:6:LEU:HD11	10:J:18:ALA:HB2	1.85	0.58
10:J:55:LYS:HG2	10:J:55:LYS:O	2.03	0.58
1:A:424:G:O2'	1:A:425:G:H5'	2.03	0.58
4:D:60:LYS:HA	4:D:202:VAL:HG22	1.85	0.58
1:A:923:A:OP1	5:E:17:ALA:HB2	2.03	0.58
12:L:123:GLU:O	12:L:123:GLU:HG3	2.02	0.58
3:C:68:HIS:HA	3:C:103:GLN:HB2	1.85	0.58
6:F:33:TYR:HA	6:F:71:ARG:NH2	2.19	0.58
8:H:11:THR:HA	8:H:14:ARG:NH1	2.18	0.58
18:R:4:LYS:N	18:R:4:LYS:HD2	2.18	0.58
18:R:72:ARG:O	18:R:73:LYS:CB	2.52	0.58
3:C:118:ARG:NH1	3:C:139:ARG:NH1	2.52	0.58
6:F:33:TYR:CD2	6:F:75:LEU:HD23	2.39	0.58
10:J:80:ILE:N	10:J:80:ILE:HD12	2.18	0.58
14:N:56:ARG:HG2	14:N:57:LYS:N	2.13	0.58
20:T:36:LEU:HD12	20:T:45:ALA:HA	1.84	0.58
1:A:1475:G:H2'	1:A:1476:G:O4'	2.03	0.58
2:B:16:LYS:HG3	2:B:34:HIS:HE1	1.69	0.58
1:A:1249:C:H4'	9:I:35:TYR:OH	2.04	0.58
1:A:1201:A:H4'	1:A:1202:G:C5'	2.34	0.58
1:A:1447:A:O2'	1:A:1452:C:OP1	2.20	0.58
1:A:460:G:C3'	1:A:461:A:H5"	2.34	0.58
1:A:49:U:C2'	1:A:50:A:H5"	2.33	0.58
3:C:38:ILE:HG22	3:C:39:ARG:N	2.18	0.58
10:J:96:ILE:N	10:J:96:ILE:HD12	2.19	0.58
20:T:49:MET:HG3	20:T:77:LEU:CD1	2.33	0.58
1:A:472:A:H2'	1:A:473:G:O4'	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:45:LEU:HD22	2:B:49:PHE:HE1	1.67	0.57
3:C:130:ARG:O	3:C:134:LYS:HG3	2.04	0.57
1:A:143:A:H2	1:A:220:G:H1	1.52	0.57
1:A:838:G:H1	1:A:848:C:H42	1.51	0.57
4:D:111:VAL:HG23	4:D:160:ASN:ND2	2.16	0.57
10:J:73:ILE:HG22	10:J:74:ASN:N	2.19	0.57
1:A:1145:C:H4'	1:A:1146:A:H5'	1.85	0.57
1:A:1230:C:O2'	1:A:1231:G:H5'	2.04	0.57
1:A:1481:U:O2'	1:A:1482:G:H5'	2.04	0.57
1:A:513:C:O2'	1:A:514:C:H5'	2.04	0.57
2:B:209:LEU:O	2:B:213:VAL:HG23	2.04	0.57
3:C:21:TRP:CZ3	3:C:31:LEU:HB2	2.40	0.57
7:G:56:GLU:O	7:G:60:VAL:HG23	2.03	0.57
15:O:5:GLU:CD	15:O:5:GLU:H	2.06	0.57
20:T:50:ARG:HH11	20:T:50:ARG:CG	2.16	0.57
1:A:1144:G:H21	1:A:1146:A:N6	2.01	0.57
1:A:1182:G:C4'	1:A:1183:A:H5'	2.30	0.57
1:A:1368:G:O2'	1:A:1369:C:H5'	2.05	0.57
1:A:922:G:H2'	1:A:923:A:C8	2.38	0.57
4:D:2:ARG:HE	4:D:2:ARG:CA	2.17	0.57
4:D:82:SER:CA	4:D:88:THR:CG2	2.77	0.57
5:E:87:LEU:HD23	5:E:116:THR:CG2	2.28	0.57
9:I:78:LEU:O	9:I:81:ALA:HB3	2.04	0.57
13:M:48:THR:HG22	13:M:50:ALA:N	2.15	0.57
16:P:12:LYS:O	16:P:13:HIS:HB2	2.05	0.57
18:R:32:THR:HG23	18:R:68:GLU:H	1.69	0.57
1:A:1004:A:H2'	1:A:1005:A:O4'	2.04	0.57
1:A:1318:A:H2'	1:A:1319:A:H5'	1.86	0.57
1:A:153:C:O2'	1:A:154:C:H5'	2.04	0.57
3:C:54:VAL:O	3:C:54:VAL:HG12	2.04	0.57
4:D:31:ALA:O	4:D:35:ARG:HB3	2.03	0.57
8:H:91:ARG:O	8:H:91:ARG:HG3	2.04	0.57
12:L:21:PRO:C	12:L:23:LEU:H	2.05	0.57
2:B:13:HIS:ND1	2:B:198:ASN:ND2	2.52	0.57
2:B:48:THR:O	2:B:52:ILE:HG12	2.03	0.57
3:C:21:TRP:CH2	3:C:31:LEU:HB2	2.39	0.57
5:E:53:LYS:HG2	5:E:57:TYR:CE2	2.40	0.57
6:F:10:LEU:CD1	6:F:59:TYR:HB3	2.29	0.57
8:H:63:LEU:N	8:H:63:LEU:HD22	2.19	0.57
12:L:22:ALA:O	12:L:23:LEU:O	2.23	0.57
1:A:838:G:H1	1:A:848:C:N4	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:LYS:HD3	2:B:189:ASP:OD2	2.05	0.57
9:I:126:LYS:CA	9:I:126:LYS:HE3	2.34	0.57
14:N:21:THR:OG1	14:N:32:VAL:HG21	2.04	0.57
17:Q:94:TYR:N	17:Q:94:TYR:CD1	2.72	0.57
17:Q:94:TYR:N	17:Q:94:TYR:HD1	2.02	0.57
1:A:664:G:OP1	18:R:49:ARG:HD2	2.04	0.57
1:A:1442:G:H2'	1:A:1442(B):A:N7	2.18	0.57
3:C:51:LEU:CD2	3:C:51:LEU:H	2.17	0.57
4:D:173:LEU:O	4:D:174:SER:CB	2.52	0.57
4:D:57:LEU:HD23	4:D:205:PHE:CZ	2.40	0.57
14:N:13:PRO:O	14:N:14:LYS:HB2	2.05	0.57
20:T:50:ARG:HH11	20:T:50:ARG:HG2	1.70	0.57
3:C:22:TYR:CD1	3:C:23:ALA:N	2.73	0.57
1:A:8:A:H5"	5:E:97:ILE:HG22	1.87	0.57
5:E:89:PRO:HD2	8:H:105:ARG:HH21	1.69	0.57
12:L:85:ARG:HH21	12:L:93:ARG:NE	1.94	0.57
13:M:58:TYR:O	13:M:62:THR:HG21	2.05	0.57
1:A:1157:A:H2'	1:A:1181:G:H22	1.69	0.57
1:A:422:C:H2'	1:A:422:C:O2	2.04	0.57
1:A:706:A:C4'	11:K:19:ILE:HD11	2.35	0.57
2:B:96:LEU:N	2:B:96:LEU:HD12	2.18	0.57
4:D:61:GLN:HA	4:D:61:GLN:NE2	2.19	0.57
5:E:123:ASN:HD22	5:E:124:PRO:N	2.01	0.57
5:E:27:LEU:HD22	5:E:39:LEU:CD2	2.35	0.57
9:I:36:PHE:HB3	9:I:42:ALA:HB2	1.86	0.57
10:J:28:SER:HB3	10:J:82:GLN:NE2	2.20	0.57
11:K:57:ASP:OD1	11:K:61:LYS:HE3	2.05	0.57
12:L:107:LYS:O	12:L:108:ASP:HB2	2.04	0.57
18:R:4:LYS:HD2	18:R:4:LYS:H	1.70	0.57
20:T:35:GLN:OE1	20:T:35:GLN:HA	2.05	0.57
1:A:1329:A:P	13:M:27:ALA:HB3	2.44	0.56
1:A:189:G:O2'	1:A:189(A):C:H5'	2.04	0.56
1:A:410:G:H2'	1:A:429:U:C5	2.40	0.56
1:A:461:A:O2'	1:A:470:C:H5'	2.04	0.56
1:A:742:G:O2'	1:A:743:U:H5'	2.05	0.56
1:A:997:U:H3'	1:A:998:G:H5"	1.86	0.56
4:D:61:GLN:NE2	4:D:64:ARG:NH1	2.49	0.56
10:J:16:ALA:O	10:J:20:LYS:HG3	2.04	0.56
1:A:972:C:OP2	10:J:55:LYS:HD2	2.05	0.56
16:P:12:LYS:HG2	16:P:13:HIS:CD2	2.40	0.56
20:T:75:SER:O	20:T:79:ARG:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:A:C5'	1:A:345:C:H5	2.18	0.56
3:C:119:VAL:O	3:C:123:ILE:HD13	2.05	0.56
4:D:101:ASP:HB3	4:D:135:PRO:CB	2.35	0.56
4:D:67:TYR:CE2	4:D:96:LEU:HB3	2.39	0.56
10:J:25:ALA:C	10:J:27:ARG:H	2.09	0.56
13:M:20:TYR:H	13:M:20:TYR:HD1	1.53	0.56
4:D:69:ILE:HG23	4:D:73:GLN:HB2	1.87	0.56
5:E:12:THR:HG23	5:E:23:ARG:O	2.05	0.56
9:I:8:ARG:HG3	9:I:13:VAL:HG22	1.86	0.56
16:P:34:GLU:OE2	16:P:55:ARG:HD3	2.05	0.56
17:Q:67:ARG:HG3	17:Q:67:ARG:HH11	1.71	0.56
1:A:420:U:H2'	1:A:422:C:H6	1.71	0.56
3:C:128:ALA:O	3:C:131:ARG:HB3	2.05	0.56
6:F:22:GLU:OE1	6:F:22:GLU:HA	2.05	0.56
10:J:96:ILE:H	10:J:96:ILE:HD12	1.70	0.56
1:A:537:G:OP1	12:L:109:ARG:NH2	2.39	0.56
12:L:23:LEU:C	12:L:25:GLY:N	2.59	0.56
23:Z:39:U:H2'	23:Z:40:C:C6	2.41	0.56
1:A:153:C:H42	1:A:168:G:H1	1.53	0.56
2:B:160:ASP:CB	2:B:199:ASP:HB2	2.33	0.56
1:A:471:G:H21	16:P:82:GLN:NE2	2.03	0.56
1:A:1047:G:H2'	1:A:1048:G:H5"	1.88	0.56
1:A:1417:G:H2'	1:A:1482:G:N2	2.20	0.56
1:A:56:U:H2'	1:A:57:G:H8	1.70	0.56
2:B:17:ARG:HH12	2:B:185:ASP:HA	1.70	0.56
2:B:211:ARG:HA	2:B:214:ASP:OD2	2.06	0.56
1:A:542:G:OP1	4:D:9:ARG:NH2	2.35	0.56
10:J:92:VAL:HG12	10:J:93:GLU:N	2.21	0.56
20:T:3:LEU:HD12	20:T:5:ALA:HB3	1.87	0.56
1:A:1001(A):G:H3'	1:A:1002:G:H8	1.71	0.56
1:A:1241:G:H2'	1:A:1242:C:H6	1.70	0.56
1:A:1276:G:C3'	1:A:1277:C:H5"	2.27	0.56
1:A:131:C:H2'	1:A:132:C:H6	1.71	0.56
1:A:1347:G:O2'	1:A:1348:U:P	2.64	0.56
4:D:120:VAL:HG22	4:D:125:ILE:HD12	1.87	0.56
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.37	0.56
1:A:1508:G:O2'	1:A:1509:C:H5'	2.06	0.56
7:G:119:ILE:HD12	7:G:119:ILE:H	1.70	0.56
18:R:24:VAL:HG13	18:R:25:LEU:HD23	1.87	0.56
20:T:93:ILE:O	20:T:95:GLY:N	2.35	0.56
21:V:23:ARG:O	21:V:24:LYS:HG2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:C:H2'	1:A:338:A:H8	1.71	0.56
2:B:80:GLU:HG3	2:B:86:TYR:HE2	1.71	0.56
2:B:91:TRP:HH2	2:B:170:GLU:CD	2.09	0.56
5:E:11:ARG:CD	5:E:22:PHE:HD2	2.17	0.56
8:H:84:ARG:HH21	8:H:86:ILE:HD11	1.71	0.56
9:I:48:PRO:O	9:I:51:ALA:HB3	2.05	0.56
12:L:122:LYS:O	12:L:122:LYS:HD2	2.06	0.56
12:L:54:VAL:O	12:L:61:GLU:HA	2.05	0.56
15:O:3:THR:HB	15:O:5:GLU:OE2	2.05	0.56
1:A:437:U:H5"	4:D:154:LEU:HD11	1.87	0.56
1:A:861:G:O2'	1:A:862:C:H5'	2.05	0.56
2:B:73:ASP:O	2:B:76:ARG:HG3	2.05	0.56
5:E:122:ARG:HG3	5:E:122:ARG:HH11	1.71	0.56
16:P:4:ILE:HG13	16:P:64:ALA:HB1	1.88	0.56
17:Q:62:ARG:HG2	17:Q:63:PRO:HD2	1.87	0.56
1:A:103:C:H2'	1:A:104:G:H5'	1.88	0.56
1:A:337:C:H2'	1:A:338:A:C8	2.41	0.56
1:A:718:G:H4'	11:K:107:ASN:ND2	2.21	0.56
12:L:24:LYS:HD3	12:L:29:ARG:HH12	1.71	0.56
12:L:23:LEU:HB2	12:L:58:SER:HB2	1.87	0.56
17:Q:63:PRO:HB3	17:Q:69:ARG:NH1	2.21	0.56
18:R:31:GLU:CD	18:R:31:GLU:N	2.58	0.56
21:V:5:ARG:HE	21:V:14:ARG:CZ	2.18	0.56
23:Z:41:C:H2'	23:Z:42:C:H5"	1.87	0.56
1:A:991:U:C4	1:A:1212:U:H1'	2.41	0.55
5:E:140:THR:HB	5:E:143:ASP:OD1	2.06	0.55
15:O:63:ARG:HH12	15:O:67:ARG:NH2	2.05	0.55
16:P:3:LYS:HD2	16:P:65:GLN:O	2.05	0.55
1:A:1314:C:O5'	19:S:5:LYS:HD3	2.05	0.55
1:A:1347:G:O2'	1:A:1348:U:OP2	2.24	0.55
1:A:586:C:O2'	1:A:587:G:H5'	2.05	0.55
19:S:36:ARG:N	19:S:36:ARG:HD2	2.16	0.55
1:A:1481:U:H2'	1:A:1482:G:C8	2.41	0.55
1:A:437:U:O2'	1:A:438:G:H5'	2.05	0.55
1:A:735:C:O2'	1:A:736:C:H5'	2.06	0.55
9:I:117:LYS:O	9:I:118:ALA:CB	2.55	0.55
10:J:32:VAL:HG13	10:J:72:ILE:CG2	2.37	0.55
12:L:86:VAL:HG11	12:L:89:LEU:HD12	1.89	0.55
19:S:16:GLU:HA	19:S:19:LEU:HD11	1.89	0.55
1:A:1126:U:H6	1:A:1280:A:N7	2.05	0.55
1:A:186:C:H2'	1:A:187:C:C6	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:G:H2'	1:A:428:G:N2	2.21	0.55
1:A:451:A:N6	1:A:481:G:H5'	2.14	0.55
1:A:524:G:H5'	1:A:525:C:OP2	2.07	0.55
7:G:144:ALA:C	7:G:146:ALA:H	2.08	0.55
8:H:82:HIS:HD2	8:H:83:ILE:N	2.04	0.55
12:L:41:PRO:HB3	12:L:88:ASP:HB3	1.88	0.55
9:I:126:LYS:HB3	13:M:125:LYS:HZ3	1.70	0.55
1:A:1245:A:H61	1:A:1292:U:H3	1.54	0.55
1:A:1402:C:O2	1:A:1500:A:N1	2.40	0.55
3:C:18:GLU:O	3:C:39:ARG:NH2	2.39	0.55
12:L:39:VAL:HG12	12:L:40:THR:H	1.71	0.55
13:M:7:GLU:OE1	13:M:7:GLU:HA	2.06	0.55
16:P:67:THR:HG22	16:P:68:ASP:N	2.21	0.55
1:A:115:G:H1'	1:A:116:A:N7	2.22	0.55
1:A:523:A:H61	12:L:88:ASP:HB2	1.71	0.55
1:A:629:G:H2'	1:A:630:G:C4'	2.37	0.55
3:C:155:ARG:O	3:C:155:ARG:HD3	2.07	0.55
4:D:193:LEU:HD22	4:D:193:LEU:N	2.21	0.55
19:S:66:VAL:HG12	19:S:67:GLY:N	2.21	0.55
1:A:1029:C:C3'	1:A:1030:C:H5"	2.37	0.55
1:A:718:G:C4'	11:K:107:ASN:ND2	2.69	0.55
3:C:133:ILE:HD11	3:C:152:VAL:CG2	2.36	0.55
5:E:122:ARG:HG3	5:E:122:ARG:NH1	2.22	0.55
20:T:93:ILE:C	20:T:95:GLY:H	2.10	0.55
1:A:1244:C:O2'	1:A:1245:A:H8	1.89	0.55
1:A:1381:U:O2'	1:A:1382:C:H5'	2.07	0.55
1:A:824:C:H2'	1:A:825:G:C8	2.41	0.55
10:J:69:LEU:O	10:J:70:VAL:HB	2.07	0.55
1:A:275:G:H5"	17:Q:13:LYS:CB	2.36	0.55
17:Q:4:VAL:HA	17:Q:58:ILE:O	2.05	0.55
18:R:21:ASN:ND2	18:R:21:ASN:C	2.59	0.55
1:A:1118:C:H2'	1:A:1119:C:H6	1.70	0.55
14:N:23:CYS:H	14:N:32:VAL:HG12	1.72	0.55
15:O:86:ILE:CG2	15:O:87:ARG:N	2.70	0.55
17:Q:58:ILE:CD1	17:Q:72:VAL:HA	2.36	0.55
1:A:1019:C:H2'	1:A:1020:U:H5'	1.88	0.55
1:A:299:G:H2'	1:A:300:A:C8	2.42	0.55
1:A:343:U:H2'	1:A:345:C:C4	2.42	0.55
1:A:564:C:C6	17:Q:30:LEU:HD11	2.42	0.55
5:E:92:PRO:HA	5:E:113:ASP:OD2	2.07	0.55
9:I:126:LYS:HA	9:I:126:LYS:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1366:C:O2'	10:J:58:ARG:NH2	2.39	0.55
13:M:22:TYR:HB3	13:M:66:GLU:H	1.71	0.55
15:O:86:ILE:O	15:O:87:ARG:CB	2.55	0.55
1:A:1014:A:H2'	1:A:1015:A:C8	2.41	0.54
1:A:1299:A:H5'	1:A:1300:G:OP2	2.06	0.54
1:A:1510:U:H2'	1:A:1511:G:C8	2.42	0.54
1:A:376:G:H5"	16:P:5:ARG:HB2	1.89	0.54
2:B:200:ASP:O	2:B:201:ALA:HB3	2.07	0.54
6:F:100:ASN:ND2	18:R:8:LYS:HG2	2.19	0.54
1:A:1031:G:O2'	1:A:1032:G:H5'	2.07	0.54
1:A:159:G:C8	1:A:159:G:H5"	2.42	0.54
1:A:30:U:H5'	1:A:31:G:OP2	2.07	0.54
1:A:5:U:H5"	1:A:5:U:O2	2.07	0.54
1:A:629:G:H2'	1:A:630:G:O4'	2.08	0.54
4:D:126:THR:HG23	4:D:146:ALA:HB3	1.88	0.54
4:D:31:ALA:C	4:D:33:GLU:N	2.60	0.54
8:H:94:TYR:O	8:H:95:VAL:HG13	2.07	0.54
13:M:10:ARG:CG	13:M:11:ASN:N	2.70	0.54
13:M:89:LEU:HD23	13:M:92:ARG:HD2	1.89	0.54
14:N:23:CYS:H	14:N:32:VAL:CG1	2.21	0.54
20:T:52:ALA:O	20:T:56:ILE:HG13	2.06	0.54
1:A:1305:G:P	21:V:1:GLY:H3	2.30	0.54
1:A:1316:G:N2	1:A:1318:A:H3'	2.23	0.54
2:B:160:ASP:HB3	2:B:163:LYS:HB2	1.88	0.54
2:B:85:PRO:HG3	2:B:149:LEU:HD13	1.88	0.54
4:D:151:SER:O	4:D:154:LEU:HB2	2.08	0.54
6:F:48:LEU:HD13	6:F:52:ILE:HG13	1.89	0.54
1:A:1030(D):A:H2'	1:A:1031:G:O4'	2.08	0.54
1:A:1286:A:H2'	1:A:1287:A:H4'	1.88	0.54
1:A:49:U:H3'	1:A:50:A:H5"	1.88	0.54
2:B:90:ARG:O	2:B:92:LEU:HD23	2.08	0.54
3:C:22:TYR:C	3:C:22:TYR:CD1	2.80	0.54
9:I:8:ARG:CG	9:I:13:VAL:HG22	2.37	0.54
1:A:251:G:HO2'	1:A:252:U:H6	1.55	0.54
1:A:746:A:O2'	1:A:747:C:H5'	2.08	0.54
2:B:38:LEU:HA	2:B:41:THR:OG1	2.07	0.54
17:Q:47:GLU:O	17:Q:48:GLU:C	2.46	0.54
17:Q:77:GLU:OE2	17:Q:80:ARG:HD2	2.07	0.54
1:A:100:C:H2'	1:A:101:A:C8	2.43	0.54
1:A:1152:A:OP1	10:J:66:HIS:ND1	2.41	0.54
1:A:1157:A:H2'	1:A:1181:G:N2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1406:U:O2'	1:A:1407:C:H5'	2.08	0.54
1:A:267:C:H2'	1:A:268:C:C6	2.43	0.54
3:C:36:GLN:HE21	14:N:46:LEU:HD13	1.72	0.54
8:H:127:LEU:HD23	8:H:127:LEU:N	2.22	0.54
1:A:1145:C:O2'	1:A:1146:A:H5'	2.07	0.54
1:A:1198:G:H2'	1:A:1199:U:C6	2.43	0.54
2:B:45:LEU:HD22	2:B:49:PHE:CE1	2.42	0.54
6:F:75:LEU:O	6:F:79:LEU:HG	2.08	0.54
6:F:99:ALA:C	6:F:101:ALA:H	2.10	0.54
8:H:119:LEU:HD12	8:H:124:ALA:CA	2.38	0.54
1:A:647:C:O2'	1:A:648:A:H5"	2.08	0.54
2:B:91:TRP:HZ2	2:B:96:LEU:HD13	1.73	0.54
6:F:13:ASN:O	6:F:14:LEU:HD23	2.08	0.54
7:G:144:ALA:O	7:G:146:ALA:N	2.39	0.54
8:H:118:VAL:O	8:H:119:LEU:HD23	2.08	0.54
9:I:126:LYS:H	9:I:126:LYS:HE3	1.72	0.54
11:K:4:VAL:HG21	11:K:30:ILE:HD13	1.89	0.54
13:M:115:THR:HG22	13:M:116:VAL:N	2.22	0.54
14:N:23:CYS:N	14:N:32:VAL:HG12	2.23	0.54
1:A:1178:G:N2	1:A:1180:A:H3'	2.22	0.54
1:A:858:G:H22	1:A:869:G:H3'	1.72	0.54
1:A:979:C:H2'	1:A:980:C:H5'	1.90	0.54
4:D:4:ILE:H	4:D:114:ARG:NH2	2.06	0.54
10:J:47:VAL:HG13	14:N:40:ARG:HB2	1.90	0.54
11:K:7:GLY:O	11:K:70:VAL:HG23	2.07	0.54
20:T:38:GLN:HA	20:T:84:LEU:HD22	1.89	0.54
1:A:1216:G:H5"	14:N:4:ALA:CB	2.38	0.54
1:A:1276:G:H3'	1:A:1277:C:C5'	2.28	0.54
1:A:1429:C:H2'	1:A:1430:C:H6	1.72	0.54
1:A:382:A:H2'	1:A:383:A:C8	2.43	0.54
1:A:778:G:O2'	1:A:779:C:H5'	2.08	0.54
1:A:77:G:O2'	1:A:78:G:H5'	2.08	0.54
1:A:806:C:O2'	1:A:807:A:H5'	2.06	0.54
2:B:212:ALA:O	2:B:216:ILE:HG12	2.08	0.54
3:C:16:ASP:HB3	3:C:20:ARG:HH12	1.73	0.54
4:D:200:GLN:HA	4:D:200:GLN:OE1	2.08	0.54
6:F:4:TYR:CE1	6:F:92:LYS:HG2	2.43	0.54
11:K:17:ASN:ND2	11:K:18:THR:N	2.53	0.54
15:O:16:ARG:HG3	15:O:16:ARG:NH1	2.20	0.54
6:F:101:ALA:HB2	18:R:13:GLU:HA	1.90	0.54
18:R:23:GLU:HA	18:R:26:LYS:HE2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:C:C2'	1:A:37:U:H5'	2.38	0.53
1:A:697:U:H2'	1:A:698:G:H5'	1.89	0.53
4:D:31:ALA:C	4:D:33:GLU:H	2.11	0.53
1:A:1048:G:C6	1:A:1210:C:N4	2.76	0.53
1:A:818:G:C2'	1:A:819:A:H5"	2.38	0.53
6:F:40:VAL:O	6:F:41:GLU:HG3	2.08	0.53
7:G:19:ASP:HB3	7:G:22:VAL:HG23	1.89	0.53
8:H:80:ILE:O	8:H:80:ILE:HG22	2.07	0.53
16:P:74:LEU:O	16:P:79:VAL:HG23	2.08	0.53
1:A:1126:U:C2'	1:A:1126:U:O2	2.56	0.53
1:A:1145:C:H4'	1:A:1146:A:C5'	2.38	0.53
1:A:629:G:H3'	1:A:630:G:H5"	1.90	0.53
1:A:862:C:O2'	1:A:863:U:H5'	2.08	0.53
2:B:96:LEU:N	2:B:96:LEU:CD1	2.71	0.53
1:A:1375:A:H4'	7:G:28:LYS:HE3	1.91	0.53
9:I:124:TYR:CD2	9:I:127:ARG:HG2	2.43	0.53
10:J:80:ILE:CD1	10:J:80:ILE:H	2.21	0.53
1:A:1314:C:H5"	19:S:5:LYS:HZ3	1.73	0.53
1:A:376:G:H2'	1:A:377:G:H8	1.73	0.53
1:A:404:U:H2'	1:A:405:U:H6	1.74	0.53
4:D:17:LYS:HA	4:D:32:MET:HG3	1.89	0.53
6:F:100:ASN:OD1	18:R:12:GLY:HA2	2.09	0.53
11:K:116:ARG:O	11:K:117:LYS:HB2	2.07	0.53
12:L:57:THR:C	12:L:59:GLY:H	2.12	0.53
13:M:65:LEU:N	13:M:65:LEU:HD12	2.23	0.53
1:A:1121:U:H2'	1:A:1122:U:C6	2.44	0.53
1:A:411:A:C4	1:A:413:G:H1'	2.43	0.53
2:B:108:ARG:NH2	2:B:112:LEU:HG	2.20	0.53
2:B:31:ASN:O	2:B:33:ILE:HG13	2.08	0.53
4:D:63:LEU:HD12	4:D:74:PHE:HZ	1.73	0.53
11:K:34:SER:H	11:K:37:VAL:HG22	1.73	0.53
12:L:105:GLY:HA3	12:L:117:GLY:O	2.09	0.53
13:M:72:GLU:O	13:M:75:ALA:HB3	2.09	0.53
16:P:22:THR:HA	16:P:33:ILE:HG13	1.90	0.53
19:S:14:LEU:HD23	19:S:14:LEU:H	1.74	0.53
20:T:58:LYS:HA	20:T:61:LYS:HG2	1.90	0.53
1:A:404:U:H2'	1:A:405:U:C6	2.44	0.53
1:A:437:U:H2'	1:A:438:G:H5'	1.90	0.53
1:A:470:C:O2'	1:A:471:G:OP1	2.27	0.53
1:A:877:C:OP1	8:H:88:LYS:HE2	2.08	0.53
2:B:123:GLU:O	2:B:124:ARG:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:PHE:HB3	2:B:38:LEU:HD11	1.91	0.53
1:A:1124:G:O2'	1:A:1145:C:N4	2.42	0.53
1:A:997:U:H2'	1:A:998:G:H5"	1.90	0.53
2:B:62:ILE:HG12	2:B:155:ALA:HB3	1.90	0.53
3:C:133:ILE:O	3:C:137:VAL:HG23	2.09	0.53
13:M:10:ARG:HG3	13:M:11:ASN:N	2.24	0.53
15:O:69:LEU:HD12	15:O:77:TYR:CB	2.38	0.53
1:A:620:C:C2	4:D:134:LEU:HD13	2.43	0.53
2:B:65:VAL:HG12	2:B:164:GLU:HG2	1.90	0.53
7:G:135:LYS:O	7:G:139:ASP:HB2	2.09	0.53
9:I:88:ASN:HB3	9:I:91:TYR:CD2	2.44	0.53
17:Q:12:ASP:OD2	17:Q:51:LYS:HG2	2.09	0.53
1:A:1264:C:H2'	1:A:1265:G:H8	1.73	0.53
1:A:1438:G:H2'	1:A:1439:C:C6	2.44	0.53
1:A:163:C:O2'	1:A:164:U:H5'	2.09	0.53
2:B:87:VAL:HG11	2:B:91:TRP:HD1	1.74	0.53
3:C:130:ARG:HH11	3:C:130:ARG:HB2	1.70	0.53
4:D:30:CYS:C	4:D:32:MET:H	2.12	0.53
7:G:153:TYR:O	7:G:155:TRP:N	2.41	0.53
10:J:6:LEU:HB2	10:J:68:ARG:HB2	1.91	0.53
15:O:84:LEU:HD13	15:O:86:ILE:HD11	1.91	0.53
1:A:818:G:H3'	1:A:819:A:C5'	2.39	0.53
2:B:198:ASN:HB3	2:B:200:ASP:O	2.09	0.53
3:C:130:ARG:HH11	3:C:130:ARG:CB	2.22	0.53
6:F:46:ARG:HB2	6:F:60:PHE:CE1	2.43	0.53
10:J:19:GLN:C	10:J:22:VAL:HG12	2.30	0.53
12:L:122:LYS:H	12:L:122:LYS:NZ	2.06	0.53
19:S:62:THR:CG2	19:S:63:GLU:N	2.72	0.53
3:C:39:ARG:O	3:C:43:GLU:HG3	2.10	0.52
3:C:57:GLU:HB2	3:C:64:ALA:CB	2.39	0.52
6:F:30:LEU:HD23	6:F:75:LEU:HD21	1.92	0.52
8:H:25:ASP:OD1	8:H:60:ARG:NE	2.42	0.52
10:J:88:LEU:N	10:J:89:PRO:CD	2.72	0.52
16:P:75:ARG:O	16:P:78:GLY:N	2.42	0.52
17:Q:3:LYS:HD2	17:Q:5:LEU:CD2	2.37	0.52
1:A:129:U:O2'	1:A:130:A:H2'	2.09	0.52
1:A:445:G:H2'	1:A:446:G:C8	2.45	0.52
1:A:652:U:O4	1:A:752:G:O2'	2.23	0.52
10:J:4:ILE:CG2	10:J:96:ILE:HG23	2.39	0.52
1:A:1284:C:C3'	1:A:1285:A:H5"	2.36	0.52
1:A:460:G:C3'	1:A:461:A:C5'	2.79	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:G:C5	1:A:731:G:H1'	2.44	0.52
2:B:53:GLU:HB3	2:B:215:LEU:CD1	2.35	0.52
3:C:153:SER:OG	3:C:154:GLY:N	2.39	0.52
3:C:34:GLU:O	3:C:37:ARG:HB2	2.10	0.52
8:H:119:LEU:HB3	8:H:123:GLU:HB3	1.92	0.52
18:R:18:ASP:OD2	18:R:21:ASN:HB2	2.08	0.52
1:A:1356:G:H2'	1:A:1357:A:C8	2.44	0.52
2:B:129:GLN:O	2:B:133:LYS:HB2	2.09	0.52
5:E:27:LEU:HD22	5:E:39:LEU:HD22	1.91	0.52
7:G:120:ALA:O	7:G:124:MET:HG3	2.09	0.52
11:K:22:ILE:HD12	11:K:62:ALA:HB2	1.92	0.52
11:K:44:ARG:HH11	11:K:44:ARG:CB	2.22	0.52
12:L:115:LYS:O	12:L:116:TYR:HB2	2.10	0.52
1:A:909:A:OP1	12:L:17:LYS:HD3	2.10	0.52
1:A:1047:G:C2'	1:A:1048:G:H5"	2.39	0.52
2:B:148:LEU:N	2:B:148:LEU:HD23	2.25	0.52
2:B:161:PRO:O	2:B:165:ALA:N	2.43	0.52
2:B:3:GLU:CD	2:B:4:LEU:H	2.12	0.52
5:E:47:VAL:O	5:E:50:ALA:HB3	2.09	0.52
6:F:67:MET:HB2	6:F:68:PRO:CD	2.40	0.52
7:G:77:ARG:HB2	7:G:155:TRP:HZ3	1.75	0.52
13:M:53:VAL:O	13:M:57:GLU:HB2	2.10	0.52
1:A:17:U:H1'	1:A:1080:A:N3	2.24	0.52
3:C:26:LYS:HA	3:C:29:ARG:HH22	1.74	0.52
7:G:47:LYS:O	7:G:50:GLN:HB3	2.09	0.52
10:J:30:ALA:C	10:J:32:VAL:N	2.62	0.52
12:L:109:ARG:NH1	12:L:112:SER:H	2.08	0.52
13:M:10:ARG:HG3	13:M:11:ASN:H	1.74	0.52
14:N:8:LYS:HD3	14:N:9:ALA:N	2.25	0.52
16:P:28:ARG:HH11	16:P:28:ARG:HG3	1.75	0.52
16:P:67:THR:CG2	16:P:68:ASP:N	2.72	0.52
17:Q:43:ALA:HA	17:Q:70:PHE:O	2.10	0.52
1:A:1309:G:O2'	1:A:1310:G:H5'	2.10	0.52
1:A:36:C:OP1	12:L:119:LYS:HE3	2.10	0.52
1:A:858:G:H5"	1:A:858:G:C8	2.40	0.52
1:A:977:A:H2'	1:A:978:A:H5"	1.90	0.52
4:D:121:ARG:NH2	4:D:133:ASP:OD2	2.43	0.52
9:I:45:ALA:HB2	9:I:73:ILE:HG23	1.92	0.52
10:J:31:GLN:HG2	10:J:31:GLN:O	2.08	0.52
12:L:46:SER:O	12:L:47:ALA:HB2	2.09	0.52
1:A:108:G:H5'	1:A:109:A:H5"	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1312:G:O2'	1:A:1313:U:H5'	2.09	0.52
4:D:154:LEU:HD23	4:D:155:GLU:N	2.24	0.52
1:A:1125:U:O4	10:J:3:ARG:NH2	2.43	0.52
10:J:3:ARG:HD2	10:J:97:LYS:HB2	1.90	0.52
13:M:93:ARG:HG3	13:M:93:ARG:HH11	1.75	0.52
14:N:22:ARG:NH1	14:N:22:ARG:HG2	2.25	0.52
15:O:13:GLU:HG3	15:O:14:PHE:CE1	2.44	0.52
21:V:8:ARG:O	21:V:12:ILE:HG12	2.10	0.52
1:A:1132:C:H2'	1:A:1133:G:C8	2.45	0.52
1:A:1442(A):G:H4'	1:A:1442(B):A:O5'	2.10	0.52
1:A:858:G:C6	1:A:869:G:C8	2.98	0.52
2:B:159:VAL:O	2:B:181:LEU:O	2.28	0.52
1:A:1112:C:O2	3:C:178:ARG:HG2	2.10	0.52
5:E:146:ARG:HB2	5:E:146:ARG:NH1	2.25	0.52
7:G:34:LYS:HD3	7:G:37:LEU:HD23	1.92	0.52
9:I:125:SER:C	9:I:127:ARG:H	2.12	0.52
1:A:251:G:O2'	1:A:252:U:H6	1.94	0.52
2:B:181:LEU:HD22	2:B:181:LEU:C	2.30	0.52
3:C:10:ARG:O	3:C:13:ILE:O	2.28	0.52
3:C:185:PHE:HD1	3:C:198:LYS:HG2	1.75	0.52
4:D:37:TYR:CD2	4:D:44:GLN:HG2	2.45	0.52
6:F:77:ARG:HA	6:F:80:ARG:HD2	1.92	0.52
13:M:34:GLU:C	13:M:36:THR:N	2.63	0.52
17:Q:86:LYS:HA	17:Q:89:ILE:HD12	1.92	0.52
17:Q:8:VAL:HG21	17:Q:83:LEU:HD12	1.92	0.52
1:A:1166:G:H5'	1:A:1168:A:OP2	2.10	0.51
1:A:1347:G:C2'	1:A:1348:U:OP2	2.58	0.51
1:A:1470:G:O2'	1:A:1471:G:H5'	2.10	0.51
1:A:1472:U:H2'	1:A:1473:A:C1'	2.40	0.51
1:A:760:G:H1	17:Q:104:ALA:HB2	1.76	0.51
5:E:72:ILE:HG12	5:E:114:ILE:HD12	1.92	0.51
5:E:96:VAL:O	5:E:103:ARG:NH2	2.41	0.51
15:O:86:ILE:CG2	15:O:87:ARG:H	2.23	0.51
19:S:14:LEU:HA	19:S:17:LYS:HE2	1.93	0.51
1:A:116:A:C8	1:A:116:A:H5'	2.39	0.51
1:A:242:C:H2'	1:A:243:A:H5'	1.92	0.51
1:A:436:C:H2'	1:A:437:U:H6	1.75	0.51
1:A:990:C:O2'	1:A:991:U:H5'	2.10	0.51
5:E:146:ARG:CB	5:E:146:ARG:NH1	2.71	0.51
6:F:32:ASN:ND2	6:F:32:ASN:N	2.58	0.51
7:G:23:THR:O	7:G:27:ASN:ND2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:119:LEU:HD12	8:H:124:ALA:CB	2.40	0.51
1:A:1279:A:H2'	1:A:1282:C:N4	2.26	0.51
1:A:220:G:O2'	1:A:221:C:H5'	2.10	0.51
1:A:848:C:O2'	1:A:849:C:H5'	2.09	0.51
4:D:56:ARG:HD2	4:D:204:GLU:HB2	1.92	0.51
6:F:10:LEU:HB3	6:F:84:ASN:O	2.10	0.51
11:K:99:VAL:HG11	18:R:69:LYS:HD3	1.91	0.51
13:M:58:TYR:CG	13:M:58:TYR:O	2.62	0.51
14:N:25:ARG:NH2	14:N:46:LEU:HD21	2.26	0.51
15:O:38:LEU:O	15:O:41:HIS:HB3	2.10	0.51
19:S:13:HIS:CD2	19:S:13:HIS:H	2.28	0.51
19:S:62:THR:H	19:S:65:MET:CG	2.24	0.51
1:A:653:A:H5'	8:H:56:LYS:CE	2.39	0.51
1:A:757:U:H2'	1:A:758:G:O4'	2.10	0.51
2:B:9:VAL:HG21	2:B:207:LEU:HD12	1.92	0.51
3:C:126:ARG:HG2	3:C:126:ARG:NH1	2.24	0.51
3:C:166:TRP:O	3:C:167:ALA:HB3	2.10	0.51
4:D:195:LEU:C	4:D:197:VAL:H	2.14	0.51
1:A:967:C:H5'	9:I:127:ARG:HB2	1.93	0.51
12:L:37:ARG:NH2	12:L:53:LYS:HZ1	2.08	0.51
14:N:32:VAL:HG23	14:N:32:VAL:O	2.11	0.51
21:V:2:LYS:HB3	21:V:13:TRP:CG	2.45	0.51
23:Z:40:C:H2'	23:Z:41:C:OP1	2.11	0.51
1:A:1057:G:H2'	1:A:1058:G:O4'	2.11	0.51
1:A:1397:C:H4'	1:A:1398:A:OP2	2.10	0.51
1:A:57:G:H2'	1:A:58:C:C6	2.46	0.51
1:A:992:U:O2	1:A:992:U:H2'	2.09	0.51
2:B:13:HIS:HD2	2:B:14:GLU:HG2	1.75	0.51
3:C:133:ILE:HD11	3:C:152:VAL:HG21	1.92	0.51
4:D:198:ASN:HD22	4:D:198:ASN:C	2.13	0.51
6:F:101:ALA:HA	18:R:13:GLU:CD	2.30	0.51
2:B:172:ARG:NH1	8:H:71:GLY:O	2.44	0.51
9:I:116:HIS:CD2	9:I:122:PRO:HA	2.46	0.51
11:K:89:GLN:HG2	11:K:95:VAL:HG21	1.93	0.51
12:L:42:LYS:O	12:L:44:PRO:HD2	2.10	0.51
1:A:1202:G:H1'	14:N:28:ARG:HD3	1.93	0.51
1:A:1392:G:N2	1:A:1502:A:H8	2.09	0.51
4:D:18:LEU:HB3	4:D:20:LEU:HG	1.93	0.51
6:F:69:GLU:HA	6:F:72:VAL:HG23	1.91	0.51
7:G:42:PHE:O	7:G:45:ALA:HB3	2.10	0.51
8:H:24:THR:HG23	8:H:24:THR:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:79:VAL:HG22	12:L:80:LEU:N	2.25	0.51
19:S:35:ARG:HH21	19:S:74:ALA:HB3	1.74	0.51
1:A:229:U:H5"	16:P:33:ILE:HD13	1.92	0.51
1:A:461:A:OP1	1:A:461:A:H8	1.93	0.51
3:C:107:ASN:ND2	3:C:143:SER:HB3	2.25	0.51
4:D:153:ASN:HA	4:D:158:ARG:HH21	1.75	0.51
4:D:195:LEU:CD2	4:D:196:PRO:HD2	2.41	0.51
5:E:86:VAL:O	5:E:116:THR:HA	2.11	0.51
1:A:1346:A:C5	7:G:9:ARG:NH1	2.78	0.51
1:A:1123:A:O3'	10:J:34:GLY:HA3	2.10	0.51
13:M:107:ARG:O	13:M:110:LYS:N	2.44	0.51
15:O:25:GLU:HG3	15:O:80:LEU:HG	1.92	0.51
1:A:106:C:C2'	1:A:107:G:H5'	2.41	0.51
1:A:1129:C:H4'	1:A:1130:A:H8	1.76	0.51
1:A:1296:C:H4'	1:A:1302:U:C4	2.46	0.51
1:A:1353:G:H2'	1:A:1354:C:H6	1.73	0.51
1:A:1372:U:O2'	1:A:1373:G:H5'	2.10	0.51
1:A:144:G:O2'	1:A:145:G:H5'	2.10	0.51
1:A:485:G:C2'	1:A:486:U:OP2	2.58	0.51
2:B:108:ARG:HH21	2:B:112:LEU:CG	2.21	0.51
3:C:34:GLU:OE2	3:C:58:ARG:NH1	2.43	0.51
4:D:29:LYS:C	4:D:31:ALA:N	2.64	0.51
4:D:35:ARG:N	4:D:36:PRO:CD	2.74	0.51
9:I:26:THR:OG1	9:I:61:TYR:HA	2.10	0.51
12:L:79:VAL:CG2	12:L:80:LEU:N	2.74	0.51
13:M:99:GLY:C	13:M:100:GLN:HG3	2.31	0.51
20:T:3:LEU:O	20:T:6:LEU:HD12	2.11	0.51
1:A:1113:C:O5'	1:A:1113:C:H6	1.94	0.51
1:A:1391:U:H2'	1:A:1392:G:H8	1.70	0.51
1:A:1394:A:C5	1:A:1501:C:H4'	2.46	0.51
2:B:217:ILE:HG21	2:B:224:VAL:CG2	2.41	0.51
4:D:144:GLU:OE2	4:D:183:LYS:HE3	2.10	0.51
11:K:48:PRO:O	11:K:51:ALA:HB3	2.11	0.51
11:K:5:ALA:HA	11:K:67:MET:HA	1.93	0.51
11:K:73:ILE:N	11:K:73:ILE:HD12	2.25	0.51
12:L:66:ILE:HD13	12:L:73:LEU:HD12	1.91	0.51
13:M:22:TYR:CE2	13:M:69:LEU:HB3	2.46	0.51
13:M:34:GLU:O	13:M:36:THR:N	2.44	0.51
18:R:11:LEU:HD21	18:R:24:VAL:CG2	2.41	0.51
18:R:24:VAL:CG1	18:R:25:LEU:N	2.73	0.51
1:A:103:C:C2'	1:A:104:G:H5'	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1109:C:H2'	1:A:1110:A:O4'	2.10	0.51
1:A:1273:G:H2'	1:A:1274:G:O4'	2.11	0.51
4:D:130:ARG:N	4:D:130:ARG:HD2	2.26	0.51
4:D:5:GLY:O	4:D:7:VAL:HG23	2.11	0.51
4:D:7:VAL:C	4:D:9:ARG:H	2.14	0.51
9:I:15:ARG:HD3	9:I:17:PHE:CZ	2.46	0.51
9:I:6:THR:H	9:I:82:ARG:CD	2.24	0.51
14:N:43:LEU:C	14:N:43:LEU:CD1	2.79	0.51
1:A:1056:U:H5'	3:C:162:ALA:CB	2.41	0.50
1:A:1428:A:H2'	1:A:1429:C:C6	2.47	0.50
1:A:448:A:C4	1:A:487:A:C2	2.99	0.50
1:A:648:A:O2'	1:A:649:G:H5'	2.11	0.50
1:A:412:A:N6	4:D:34:ARG:HB3	2.24	0.50
5:E:1:ASP:CG	5:E:2:PHE:H	2.15	0.50
9:I:4:TYR:HE2	9:I:15:ARG:HG2	1.75	0.50
10:J:26:ARG:O	10:J:27:ARG:HG3	2.11	0.50
10:J:36:ILE:HB	10:J:69:LEU:HB3	1.92	0.50
20:T:33:ALA:HB2	20:T:48:ILE:HG22	1.92	0.50
21:V:16:THR:O	21:V:21:ARG:HD3	2.11	0.50
1:A:1040:U:H2'	1:A:1041:A:H8	1.75	0.50
1:A:1166:G:H3'	1:A:1168:A:H5"	1.93	0.50
1:A:1426:C:O2'	1:A:1427:U:H5'	2.10	0.50
1:A:149:A:H2'	1:A:150:C:C6	2.46	0.50
2:B:128:GLU:HG2	2:B:132:LEU:CD1	2.42	0.50
2:B:86:TYR:CD1	2:B:145:GLY:HA3	2.46	0.50
3:C:107:ASN:HD21	3:C:143:SER:CB	2.24	0.50
3:C:78:ARG:HH21	3:C:81:GLU:HG2	1.76	0.50
7:G:115:ALA:O	7:G:119:ILE:HD12	2.10	0.50
10:J:14:LEU:C	10:J:16:ALA:N	2.65	0.50
17:Q:103:LYS:HZ3	17:Q:103:LYS:HB3	1.76	0.50
18:R:21:ASN:O	18:R:24:VAL:HG12	2.11	0.50
20:T:43:GLU:H	20:T:92:LEU:HD12	1.76	0.50
1:A:1475:G:H3'	1:A:1476:G:H5"	1.92	0.50
1:A:321:A:O2'	1:A:322:C:H5'	2.10	0.50
1:A:411:A:N3	1:A:413:G:H1'	2.26	0.50
1:A:501:C:H2'	1:A:502:G:C8	2.45	0.50
2:B:105:ARG:HB3	2:B:143:LEU:HD11	1.92	0.50
4:D:157:ILE:HD12	4:D:157:ILE:N	2.25	0.50
6:F:99:ALA:C	6:F:101:ALA:N	2.64	0.50
8:H:10:LEU:CD2	8:H:83:ILE:HD11	2.41	0.50
1:A:1123:A:H4'	10:J:35:PRO:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:14:SER:HB3	11:K:17:ASN:O	2.11	0.50
12:L:36:VAL:O	12:L:36:VAL:HG12	2.11	0.50
13:M:106:ALA:O	13:M:110:LYS:HG3	2.12	0.50
15:O:17:PHE:HB2	15:O:18:PRO:HD2	1.93	0.50
15:O:86:ILE:C	15:O:87:ARG:HD2	2.31	0.50
18:R:2:SER:O	18:R:3:ARG:HD3	2.10	0.50
1:A:1138:G:C8	1:A:1140:C:H1'	2.46	0.50
1:A:1374:A:OP1	7:G:35:LYS:HE3	2.12	0.50
1:A:1394:A:C6	1:A:1501:C:H4'	2.46	0.50
26:A:2800:RPO:HAU	26:A:2800:RPO:H6	1.93	0.50
1:A:640:A:O2'	1:A:641:U:H5'	2.11	0.50
1:A:818:G:O2'	1:A:819:A:H5"	2.12	0.50
2:B:143:LEU:O	2:B:147:ARG:HB2	2.11	0.50
3:C:76:ILE:O	3:C:82:ARG:HB3	2.11	0.50
8:H:103:VAL:CG2	8:H:110:ALA:HB2	2.42	0.50
8:H:20:TYR:CE1	8:H:76:PRO:HG2	2.46	0.50
12:L:24:LYS:C	12:L:26:ALA:N	2.54	0.50
12:L:82:ARG:HG3	12:L:82:ARG:HH11	1.76	0.50
1:A:1106:G:OP1	3:C:171:ARG:HD3	2.11	0.50
1:A:714:G:H2'	1:A:715:A:C8	2.46	0.50
5:E:135:LEU:C	5:E:137:GLN:H	2.14	0.50
13:M:10:ARG:HA	13:M:44:VAL:HB	1.93	0.50
13:M:121:LYS:O	13:M:122:ALA:HB2	2.11	0.50
6:F:100:ASN:ND2	18:R:8:LYS:O	2.44	0.50
3:C:13:ILE:HG22	3:C:14:THR:N	2.11	0.50
3:C:155:ARG:N	3:C:162:ALA:HA	2.25	0.50
3:C:171:ARG:HH12	3:C:173:PRO:HG3	1.76	0.50
5:E:118:GLU:O	5:E:119:LEU:HD23	2.11	0.50
9:I:126:LYS:N	9:I:126:LYS:HE3	2.26	0.50
12:L:24:LYS:HD3	12:L:29:ARG:HH22	1.75	0.50
1:A:1042:G:O2'	1:A:1043:C:H5'	2.12	0.50
1:A:159:G:H4'	1:A:160:A:OP2	2.11	0.50
1:A:460:G:H3'	1:A:461:A:H5'	1.88	0.50
1:A:858:G:N2	1:A:869:G:H3'	2.27	0.50
1:A:953:G:H1'	13:M:124:ARG:CA	2.33	0.50
2:B:217:ILE:O	2:B:219:ALA:N	2.45	0.50
2:B:76:ARG:HG2	2:B:76:ARG:HH11	1.76	0.50
3:C:59:ALA:O	3:C:61:ASP:N	2.45	0.50
4:D:104:VAL:CG2	4:D:125:ILE:HD13	2.34	0.50
5:E:78:VAL:HG21	5:E:133:GLU:HB3	1.94	0.50
9:I:126:LYS:O	13:M:125:LYS:NZ	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:19:ARG:O	9:I:59:ASP:N	2.45	0.50
9:I:57:ARG:O	9:I:57:ARG:HG2	2.12	0.50
10:J:75:PRO:O	10:J:76:ASN:O	2.30	0.50
13:M:64:LYS:HZ2	13:M:72:GLU:HB2	1.77	0.50
13:M:76:ASN:O	13:M:79:ARG:N	2.45	0.50
18:R:1:PRO:O	18:R:3:ARG:HG2	2.12	0.50
1:A:1258:G:H2'	1:A:1259:C:C6	2.47	0.50
1:A:1308:U:OP1	13:M:97:VAL:N	2.33	0.50
1:A:154:C:H2'	1:A:155:C:H6	1.76	0.50
1:A:443:C:H2'	1:A:444:C:C6	2.47	0.50
1:A:807:A:H2'	1:A:808:C:C6	2.47	0.50
1:A:841:U:H3'	1:A:848:C:O4'	2.12	0.50
3:C:127:PHE:HB3	3:C:131:ARG:NH1	2.27	0.50
3:C:27:GLN:N	3:C:27:GLN:OE1	2.45	0.50
4:D:21:LYS:O	4:D:112:SER:HB3	2.12	0.50
5:E:4:GLU:HA	5:E:29:VAL:O	2.11	0.50
17:Q:75:LEU:HD23	17:Q:75:LEU:C	2.32	0.50
19:S:21:LEU:HB3	19:S:27:LYS:HB2	1.93	0.50
1:A:420:U:H2'	1:A:422:C:C6	2.47	0.50
1:A:647:C:C2'	1:A:648:A:C5'	2.77	0.50
1:A:752:G:OP2	1:A:752:G:H8	1.93	0.50
4:D:42:HIS:O	4:D:44:GLN:N	2.45	0.50
7:G:115:ALA:HA	7:G:118:ARG:CZ	2.41	0.50
7:G:56:GLU:OE1	7:G:57:PRO:HD2	2.11	0.50
8:H:119:LEU:HD12	8:H:124:ALA:HB2	1.93	0.50
13:M:21:ILE:O	13:M:22:TYR:O	2.29	0.50
14:N:10:LYS:C	14:N:12:THR:H	2.14	0.50
15:O:28:VAL:HG12	15:O:84:LEU:CD1	2.41	0.50
1:A:1149:C:OP1	9:I:13:VAL:HG21	2.11	0.49
1:A:629:G:C3'	1:A:630:G:H5"	2.42	0.49
2:B:172:ARG:O	8:H:71:GLY:HA2	2.12	0.49
2:B:18:TRP:N	2:B:18:TRP:CD1	2.78	0.49
3:C:99:ALA:O	3:C:100:LEU:CB	2.57	0.49
12:L:64:ALA:CB	12:L:81:ILE:HD11	2.41	0.49
13:M:93:ARG:NH1	13:M:93:ARG:HG3	2.27	0.49
1:A:184:G:O4'	1:A:224:C:H4'	2.12	0.49
2:B:109:LEU:HD22	2:B:147:ARG:HH21	1.77	0.49
2:B:159:VAL:O	2:B:161:PRO:HD3	2.12	0.49
3:C:50:GLY:O	3:C:69:VAL:HG13	2.13	0.49
5:E:135:LEU:O	5:E:137:GLN:N	2.45	0.49
5:E:140:THR:HG23	5:E:141:LYS:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:64:GLU:O	5:E:66:PRO:HD3	2.12	0.49
6:F:69:GLU:HA	6:F:72:VAL:CG2	2.41	0.49
9:I:45:ALA:HB1	9:I:76:ILE:HG22	1.94	0.49
10:J:32:VAL:HG22	10:J:72:ILE:HG21	1.94	0.49
14:N:10:LYS:C	14:N:12:THR:N	2.66	0.49
1:A:106:C:O2'	1:A:107:G:H5'	2.12	0.49
1:A:1346:A:C6	7:G:9:ARG:NH1	2.81	0.49
1:A:1441:G:H4'	1:A:1442:G:C5	2.47	0.49
1:A:428:G:OP2	4:D:6:PRO:HG2	2.12	0.49
1:A:91:C:H2'	1:A:92:C:H6	1.78	0.49
2:B:10:HIS:HB2	2:B:198:ASN:CG	2.33	0.49
6:F:23:LYS:NZ	6:F:42:GLU:OE1	2.42	0.49
10:J:89:PRO:HB2	10:J:92:VAL:HB	1.93	0.49
18:R:38:ARG:HA	18:R:48:GLN:OE1	2.12	0.49
19:S:29:LEU:O	19:S:30:ILE:HD13	2.12	0.49
20:T:80:LYS:NZ	20:T:80:LYS:HB2	2.28	0.49
23:Z:28:G:H4'	23:Z:29:G:O5'	2.12	0.49
3:C:106:GLN:H	3:C:106:GLN:NE2	2.10	0.49
4:D:80:GLU:O	4:D:84:LYS:HG3	2.12	0.49
6:F:98:LEU:HD13	6:F:101:ALA:CB	2.42	0.49
9:I:117:LYS:HG2	9:I:120:ARG:HB3	1.94	0.49
12:L:6:LEU:O	12:L:10:GLY:N	2.45	0.49
14:N:55:VAL:O	14:N:55:VAL:HG12	2.12	0.49
17:Q:27:PRO:HA	17:Q:34:VAL:HA	1.93	0.49
1:A:216:G:O2'	1:A:217:C:P	2.70	0.49
2:B:80:GLU:C	2:B:82:ALA:H	2.16	0.49
3:C:69:VAL:C	3:C:105:VAL:HG23	2.33	0.49
5:E:72:ILE:HG23	5:E:73:PRO:HD2	1.93	0.49
1:A:1486:G:H2'	1:A:1487:G:O4'	2.13	0.49
1:A:625:G:H2'	1:A:626:U:C6	2.48	0.49
1:A:895:G:H2'	1:A:896:C:C6	2.47	0.49
1:A:918:A:H2'	1:A:919:A:C8	2.48	0.49
2:B:7:ALA:HA	2:B:11:PHE:HD2	1.77	0.49
2:B:92:LEU:N	2:B:92:LEU:CD2	2.74	0.49
5:E:123:ASN:HD22	5:E:123:ASN:C	2.15	0.49
1:A:1072:G:O6	1:A:1102:A:N6	2.46	0.49
1:A:1187:G:P	9:I:112:LYS:HZ2	2.36	0.49
1:A:320:C:H2'	1:A:321:A:C8	2.48	0.49
6:F:80:ARG:NH1	6:F:88:VAL:HB	2.28	0.49
9:I:47:GLU:OE1	9:I:50:ARG:HD2	2.13	0.49
11:K:113:LYS:O	11:K:116:ARG:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:47:THR:HG23	11:K:50:ALA:H	1.78	0.49
12:L:106:VAL:HG23	12:L:116:TYR:HB3	1.95	0.49
1:A:34:C:H1'	12:L:28:PHE:CZ	2.48	0.49
1:A:953:G:C1'	13:M:124:ARG:HA	2.32	0.49
13:M:50:ALA:O	13:M:54:ARG:HG3	2.13	0.49
16:P:45:THR:OG1	16:P:46:PRO:HD2	2.12	0.49
1:A:1142:G:H2'	1:A:1143:G:O4'	2.13	0.49
1:A:1216:G:O2'	1:A:1217:C:H5'	2.13	0.49
3:C:171:ARG:HH11	3:C:171:ARG:HB3	1.77	0.49
9:I:65:ARG:HH11	9:I:65:ARG:HG3	1.77	0.49
1:A:1119:C:O2'	1:A:1120:G:H5'	2.13	0.49
1:A:837:G:H1	1:A:849:C:H42	1.60	0.49
1:A:8:A:C6	4:D:208:ARG:HA	2.47	0.49
3:C:107:ASN:HD21	3:C:143:SER:HB3	1.77	0.49
3:C:21:TRP:CB	3:C:58:ARG:HB2	2.42	0.49
10:J:36:ILE:HB	10:J:69:LEU:CB	2.43	0.49
6:F:7:ASN:HD21	18:R:19:TYR:HE2	1.61	0.49
19:S:27:LYS:HG2	19:S:28:ARG:H	1.77	0.49
20:T:67:LYS:HZ3	20:T:67:LYS:HB2	1.78	0.49
1:A:1121:U:H2'	1:A:1122:U:H6	1.77	0.49
1:A:1170:A:H2'	1:A:1171:G:O4'	2.13	0.49
1:A:401:C:H1'	1:A:622:A:H1'	1.94	0.49
17:Q:89:ILE:O	17:Q:92:GLN:HB3	2.13	0.49
21:V:9:ARG:HB2	21:V:9:ARG:CZ	2.43	0.49
1:A:1105:A:H2'	1:A:1106:G:C8	2.48	0.48
1:A:328:C:O2	1:A:328:C:C2'	2.60	0.48
1:A:389:A:N3	1:A:389:A:H2'	2.28	0.48
1:A:449:C:O2	16:P:42:ARG:HG2	2.12	0.48
1:A:939:G:H2'	1:A:940:C:C6	2.47	0.48
2:B:75:VAL:HG22	2:B:209:LEU:HD11	1.94	0.48
3:C:125:ARG:HB3	3:C:127:PHE:CE1	2.47	0.48
5:E:14:ARG:HD3	5:E:21:ARG:O	2.12	0.48
6:F:44:GLY:HA3	6:F:59:TYR:CE1	2.49	0.48
7:G:92:PRO:HG2	7:G:93:ARG:H	1.78	0.48
10:J:27:ARG:CB	10:J:27:ARG:HH11	2.20	0.48
10:J:72:ILE:HG13	10:J:72:ILE:O	2.13	0.48
13:M:97:VAL:HG23	13:M:109:ARG:NH1	2.27	0.48
13:M:20:TYR:N	13:M:20:TYR:CD1	2.81	0.48
13:M:18:LEU:O	13:M:21:ILE:HG13	2.13	0.48
15:O:69:LEU:HD12	15:O:77:TYR:CA	2.43	0.48
19:S:12:ASP:O	19:S:13:HIS:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1288:A:H2'	1:A:1289:A:C8	2.48	0.48
1:A:1390:U:H2'	1:A:1391:U:C6	2.48	0.48
1:A:1479:C:C2'	1:A:1480:G:H5"	2.29	0.48
1:A:382:A:C2	1:A:383:A:C4	3.01	0.48
1:A:781:A:H5'	1:A:782:A:OP2	2.13	0.48
1:A:572:A:H5"	1:A:917:G:H4'	1.94	0.48
2:B:151:ARG:O	2:B:152:LEU:C	2.51	0.48
2:B:17:ARG:HH12	2:B:185:ASP:CA	2.26	0.48
3:C:154:GLY:O	3:C:155:ARG:CB	2.61	0.48
4:D:11:CYS:SG	4:D:18:LEU:HB2	2.53	0.48
10:J:13:THR:HG23	10:J:92:VAL:HG22	1.95	0.48
10:J:32:VAL:C	10:J:34:GLY:H	2.16	0.48
12:L:50:LYS:N	12:L:50:LYS:HD2	2.29	0.48
1:A:969:A:N1	13:M:125:LYS:OXT	2.46	0.48
19:S:29:LEU:HD23	19:S:47:THR:HG22	1.94	0.48
19:S:64:ASN:ND2	19:S:65:MET:N	2.58	0.48
19:S:79:TYR:O	19:S:81:GLY:N	2.46	0.48
1:A:1140:C:H2'	1:A:1140:C:O2	2.12	0.48
1:A:539:A:H2'	1:A:540:G:C8	2.48	0.48
3:C:190:THR:HG21	3:C:192:TYR:CE1	2.48	0.48
3:C:5:HIS:CD2	3:C:7:ILE:HB	2.47	0.48
3:C:5:HIS:CD2	3:C:7:ILE:H	2.32	0.48
6:F:48:LEU:HD13	6:F:52:ILE:CG1	2.44	0.48
9:I:7:GLY:CA	9:I:78:LEU:HD12	2.39	0.48
10:J:80:ILE:HG22	10:J:80:ILE:O	2.13	0.48
19:S:51:TYR:HA	19:S:55:GLN:O	2.13	0.48
1:A:1207:G:O2'	1:A:1208:C:H5'	2.13	0.48
1:A:1289:A:H5'	1:A:1290:G:OP2	2.12	0.48
1:A:271:C:O2'	1:A:272:C:H5'	2.13	0.48
1:A:818:G:C3'	1:A:819:A:C5'	2.91	0.48
1:A:97:G:O2'	1:A:98:G:H5'	2.13	0.48
2:B:2:LYS:HD2	2:B:2:LYS:C	2.34	0.48
2:B:72:GLN:O	2:B:88:ASN:ND2	2.47	0.48
3:C:173:PRO:O	3:C:175:HIS:N	2.46	0.48
3:C:35:ASP:OD1	3:C:56:ILE:HD12	2.12	0.48
3:C:46:LEU:HD12	3:C:46:LEU:N	2.28	0.48
4:D:123:GLY:HA3	4:D:131:ARG:HD2	1.94	0.48
5:E:148:ARG:NH2	8:H:107:LEU:O	2.47	0.48
6:F:50:TYR:CE1	18:R:62:GLY:HA2	2.48	0.48
17:Q:77:GLU:OE1	17:Q:80:ARG:HD2	2.13	0.48
20:T:4:SER:HA	20:T:6:LEU:CD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1141:C:HO2'	1:A:1142:G:H5'	1.79	0.48
1:A:8:A:H3'	1:A:8:A:OP1	2.13	0.48
3:C:149:LYS:HG2	3:C:150:VAL:N	2.27	0.48
3:C:46:LEU:CD1	3:C:46:LEU:H	2.27	0.48
4:D:30:CYS:O	4:D:30:CYS:SG	2.71	0.48
8:H:60:ARG:CG	8:H:60:ARG:NH1	2.76	0.48
13:M:4:ALA:O	13:M:5:GLY:C	2.52	0.48
13:M:7:GLU:C	13:M:8:ILE:HD12	2.34	0.48
14:N:44:ARG:HG3	14:N:44:ARG:NH1	2.27	0.48
23:Z:28:G:H8	23:Z:28:G:HO2'	1.61	0.48
1:A:488:C:O2'	1:A:489:C:H5'	2.13	0.48
1:A:49:U:O2'	1:A:50:A:H5"	2.13	0.48
1:A:521:G:OP2	12:L:50:LYS:HE2	2.14	0.48
1:A:644:G:O2'	1:A:645:C:H5'	2.13	0.48
5:E:68:GLN:O	5:E:69:ASN:CB	2.61	0.48
7:G:16:VAL:HG12	7:G:17:TYR:CD1	2.48	0.48
1:A:1056:U:H5'	3:C:162:ALA:HB2	1.96	0.48
1:A:1277:C:H3'	1:A:1277:C:H6	1.77	0.48
1:A:946:A:H2'	1:A:947:G:H8	1.72	0.48
1:A:986:A:H2'	1:A:987:G:C8	2.49	0.48
4:D:2:ARG:HA	4:D:2:ARG:NE	2.25	0.48
7:G:41:ILE:HD12	7:G:115:ALA:HB3	1.96	0.48
9:I:6:THR:H	9:I:82:ARG:HD2	1.79	0.48
9:I:3:TYR:HB3	9:I:86:GLN:HB2	1.96	0.48
10:J:64:ARG:HD3	10:J:66:HIS:CE1	2.48	0.48
13:M:104:THR:O	13:M:105:ASN:C	2.51	0.48
13:M:115:THR:CG2	13:M:116:VAL:N	2.77	0.48
16:P:1:MET:O	16:P:24:ALA:HB2	2.14	0.48
1:A:1090:U:H2'	1:A:1091:U:H6	1.78	0.48
1:A:1420:C:H2'	1:A:1421:G:C8	2.48	0.48
1:A:280:C:H4'	1:A:281:G:OP2	2.13	0.48
1:A:628:G:H2'	1:A:629:G:C8	2.48	0.48
1:A:818:G:H3'	1:A:819:A:H5"	1.96	0.48
1:A:945:G:H2'	1:A:945:G:N3	2.29	0.48
2:B:200:ASP:O	2:B:201:ALA:CB	2.62	0.48
4:D:7:VAL:HG13	4:D:20:LEU:HD13	1.96	0.48
8:H:134:ILE:HG22	8:H:135:CYS:SG	2.52	0.48
9:I:112:LYS:HD3	9:I:118:ALA:HA	1.96	0.48
9:I:55:LEU:HD23	9:I:55:LEU:O	2.13	0.48
9:I:92:ARG:HG3	9:I:92:ARG:NH1	2.29	0.48
1:A:275:G:C5'	17:Q:13:LYS:HB3	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:62:THR:HB	19:S:64:ASN:HD21	1.78	0.48
20:T:19:ASN:O	20:T:20:LYS:C	2.52	0.48
1:A:1020:U:H2'	1:A:1021:G:C5'	2.32	0.48
1:A:1118:C:H2'	1:A:1119:C:C6	2.49	0.48
1:A:1126:U:C6	1:A:1280:A:N7	2.81	0.48
1:A:994:A:N7	1:A:1216:G:H4'	2.29	0.48
1:A:148:G:C8	1:A:148:G:H5"	2.49	0.48
1:A:815:A:O2'	1:A:1527:C:H1'	2.14	0.48
2:B:134:HIS:CA	2:B:137:GLU:HG2	2.42	0.48
3:C:133:ILE:CD1	3:C:152:VAL:HG23	2.44	0.48
4:D:63:LEU:HD12	4:D:74:PHE:CZ	2.47	0.48
7:G:5:ARG:O	7:G:6:ALA:C	2.52	0.48
13:M:67:GLY:HA2	13:M:70:ARG:HD2	1.96	0.48
16:P:55:ARG:O	16:P:58:TYR:HB3	2.14	0.48
18:R:24:VAL:HG13	18:R:25:LEU:N	2.28	0.48
1:A:1002:G:H2'	1:A:1003:G:C8	2.48	0.48
1:A:407:G:O2'	4:D:115:GLN:HG3	2.14	0.48
6:F:35:ALA:HA	6:F:67:MET:HB3	1.94	0.48
7:G:109:GLN:OE1	7:G:109:GLN:HA	2.14	0.48
17:Q:25:GLN:O	17:Q:26:PHE:HB3	2.13	0.48
20:T:23:LYS:HE3	20:T:64:THR:HG22	1.96	0.48
1:A:1105:A:H2'	1:A:1106:G:H8	1.79	0.47
1:A:1468:A:H2'	1:A:1469:G:O4'	2.14	0.47
1:A:245:C:O2'	1:A:246:A:H5"	2.14	0.47
1:A:334:C:H2'	1:A:335:C:C6	2.49	0.47
1:A:456:C:H2'	1:A:457:C:C6	2.49	0.47
1:A:984:C:H2'	1:A:985:C:H6	1.78	0.47
2:B:126:LYS:O	2:B:130:VAL:HG23	2.14	0.47
2:B:156:ILE:HG22	2:B:158:VAL:HG13	1.95	0.47
2:B:37:ASP:OD1	2:B:39:GLN:HB2	2.14	0.47
2:B:47:ARG:HH12	2:B:193:TYR:HA	1.78	0.47
2:B:79:ALA:CB	2:B:86:TYR:HD2	2.26	0.47
3:C:21:TRP:CE3	3:C:21:TRP:O	2.67	0.47
6:F:62:TRP:CG	18:R:20:ARG:NH1	2.82	0.47
17:Q:44:HIS:ND1	17:Q:68:LYS:NZ	2.42	0.47
20:T:66:HIS:O	20:T:67:LYS:HB3	2.13	0.47
1:A:1087:G:N2	1:A:1099:G:H1'	2.29	0.47
1:A:1131:G:H2'	1:A:1132:C:C6	2.48	0.47
1:A:1168:A:H3'	1:A:1169:A:C8	2.49	0.47
1:A:189(E):U:O2'	1:A:189(F):U:H5'	2.14	0.47
2:B:53:GLU:HA	2:B:56:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:42:LEU:HD13	3:C:67:VAL:HG21	1.95	0.47
5:E:6:MET:HA	5:E:28:VAL:HG23	1.96	0.47
6:F:41:GLU:HB2	6:F:62:TRP:HB3	1.96	0.47
7:G:94:ARG:CZ	7:G:98:LEU:HD11	2.44	0.47
10:J:88:LEU:H	10:J:89:PRO:CD	2.26	0.47
17:Q:65:SER:OG	17:Q:68:LYS:HB2	2.14	0.47
1:A:1189:C:P	10:J:49:ARG:NH2	2.85	0.47
2:B:128:GLU:HG2	2:B:132:LEU:HD11	1.96	0.47
5:E:72:ILE:HD12	5:E:138:LEU:CD1	2.44	0.47
11:K:100:ASP:OD2	18:R:73:LYS:HE3	2.13	0.47
13:M:116:VAL:HG12	13:M:117:ALA:N	2.21	0.47
20:T:17:LEU:O	20:T:17:LEU:HD12	2.14	0.47
20:T:77:LEU:O	20:T:81:VAL:HG23	2.13	0.47
20:T:79:ARG:HH11	20:T:79:ARG:HG2	1.79	0.47
1:A:184:G:C4'	1:A:224:C:H4'	2.44	0.47
1:A:36:C:H2'	1:A:37:U:H5'	1.97	0.47
1:A:89:C:O5'	1:A:89:C:H6	1.96	0.47
7:G:17:TYR:CE2	7:G:58:LEU:HB2	2.49	0.47
2:B:173:LYS:HA	8:H:72:PRO:HD3	1.97	0.47
11:K:86:ARG:HH11	11:K:86:ARG:HG2	1.78	0.47
17:Q:2:LYS:HB3	17:Q:60:GLU:HB3	1.96	0.47
1:A:663:A:H5"	18:R:46:LYS:HE3	1.96	0.47
1:A:1014:A:C2	1:A:1219:U:H1'	2.49	0.47
1:A:1392:G:H21	1:A:1502:A:H8	1.61	0.47
1:A:519:C:H2'	1:A:520:A:C8	2.50	0.47
1:A:721:G:OP1	1:A:721:G:H8	1.96	0.47
1:A:858:G:C5	1:A:869:G:N7	2.82	0.47
1:A:983:A:H5'	1:A:984:C:OP2	2.13	0.47
2:B:17:ARG:O	2:B:18:TRP:O	2.32	0.47
6:F:78:GLU:OE1	6:F:78:GLU:HA	2.15	0.47
11:K:22:ILE:CD1	11:K:62:ALA:HB2	2.45	0.47
1:A:707:C:OP1	11:K:75:ARG:HD2	2.15	0.47
10:J:47:VAL:HG11	14:N:40:ARG:O	2.15	0.47
16:P:42:ARG:C	16:P:43:LYS:HG3	2.35	0.47
19:S:7:GLY:O	19:S:9:PHE:N	2.47	0.47
20:T:46:LEU:O	20:T:49:MET:HB3	2.14	0.47
1:A:501:C:H1'	1:A:549:C:H1'	1.95	0.47
1:A:541:G:O2'	1:A:542:G:H5'	2.15	0.47
2:B:217:ILE:C	2:B:219:ALA:N	2.68	0.47
8:H:112:LEU:HD11	8:H:114:THR:HG22	1.95	0.47
8:H:50:ARG:O	8:H:51:VAL:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:61:GLN:HE21	15:O:61:GLN:HA	1.79	0.47
19:S:20:GLU:C	19:S:22:ASN:H	2.16	0.47
19:S:31:LYS:HA	19:S:49:ALA:HB3	1.96	0.47
1:A:1544:U:H4'	22:W:1:U:O5'	2.14	0.47
1:A:1402:C:H2'	1:A:1403:C:O4'	2.14	0.47
1:A:1060:C:H5"	10:J:49:ARG:HB3	1.97	0.47
14:N:35:PHE:C	14:N:35:PHE:CD1	2.88	0.47
18:R:32:THR:C	18:R:34:LYS:H	2.17	0.47
20:T:23:LYS:O	20:T:27:LYS:HG3	2.15	0.47
21:V:13:TRP:C	21:V:15:GLY:H	2.18	0.47
1:A:1418:A:N6	1:A:1482:G:O2'	2.47	0.47
1:A:168:G:C2	1:A:169:C:C5	3.03	0.47
1:A:402:G:C3'	1:A:403:C:H5"	2.45	0.47
1:A:745:C:H5"	1:A:851:G:O2'	2.15	0.47
3:C:172:VAL:O	3:C:174:LEU:N	2.37	0.47
3:C:98:VAL:HG23	3:C:99:ALA:O	2.15	0.47
4:D:157:ILE:CD1	4:D:157:ILE:N	2.78	0.47
9:I:42:ALA:HA	9:I:73:ILE:HD13	1.97	0.47
16:P:71:ARG:HD3	16:P:75:ARG:NH2	2.30	0.47
1:A:1118:C:H1'	1:A:1179:A:C4	2.49	0.47
1:A:1314:C:H5"	19:S:5:LYS:HZ2	1.80	0.47
1:A:1491:G:O2'	26:A:2800:RPO:HAM	2.14	0.47
1:A:414:A:H2'	1:A:415:A:H8	1.80	0.47
1:A:495:A:H4'	1:A:496:A:OP1	2.14	0.47
1:A:715:A:H2'	1:A:716:A:H8	1.80	0.47
1:A:96:U:O2'	1:A:97:G:H5'	2.15	0.47
6:F:47:ARG:NE	6:F:47:ARG:N	2.57	0.47
9:I:69:LYS:O	9:I:73:ILE:HG13	2.14	0.47
11:K:49:TYR:CE2	11:K:53:LEU:HD11	2.50	0.47
19:S:8:VAL:CG1	19:S:38:THR:HG21	2.45	0.47
1:A:1004:A:H8	1:A:1036:G:H22	1.62	0.47
1:A:1106:G:H5"	3:C:171:ARG:HG2	1.97	0.47
1:A:1014:A:H2	1:A:1219:U:O2	1.97	0.47
1:A:1245:A:N6	1:A:1292:U:H3	2.13	0.47
1:A:1245:A:H2'	1:A:1246:C:C6	2.50	0.47
1:A:1264:C:H2'	1:A:1265:G:C8	2.50	0.47
1:A:390:C:H2'	1:A:391:G:H8	1.78	0.47
1:A:591:U:H2'	1:A:592:G:H8	1.80	0.47
1:A:958:A:C5'	1:A:959:A:OP2	2.61	0.47
3:C:178:ARG:NH1	3:C:206:VAL:HG22	2.30	0.47
1:A:932:C:C6	7:G:2:ARG:HD3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:20:LYS:NZ	10:J:88:LEU:N	2.61	0.47
10:J:4:ILE:HD11	10:J:70:VAL:HG11	1.96	0.47
12:L:115:LYS:O	12:L:116:TYR:CB	2.62	0.47
18:R:44:SER:O	18:R:45:GLY:C	2.53	0.47
1:A:1095:U:H2'	1:A:1096:C:C6	2.49	0.47
1:A:130:A:O2'	1:A:131:C:H5"	2.15	0.47
1:A:345:C:H4'	1:A:346:G:C5'	2.45	0.47
1:A:586:C:C2'	1:A:587:G:H5'	2.45	0.47
2:B:213:VAL:O	2:B:216:ILE:HB	2.14	0.47
3:C:66:THR:HG23	3:C:101:ASN:HB2	1.96	0.47
1:A:1191:A:P	3:C:2:ASN:HD22	2.38	0.47
1:A:921:U:O2'	5:E:15:MET:O	2.24	0.47
5:E:37:VAL:HG21	5:E:109:ALA:HB2	1.97	0.47
6:F:30:LEU:HB3	6:F:35:ALA:CB	2.45	0.47
6:F:39:LYS:HB2	6:F:39:LYS:NZ	2.29	0.47
9:I:112:LYS:H	9:I:118:ALA:HA	1.80	0.47
13:M:81:MET:CE	13:M:91:HIS:HB3	2.45	0.47
1:A:1292:U:H2'	1:A:1293:G:C8	2.50	0.46
1:A:146:G:H2'	1:A:147:G:C5'	2.30	0.46
1:A:173:U:H6	1:A:198:G:HO2'	1.61	0.46
1:A:538:G:OP2	12:L:111:LYS:HD2	2.15	0.46
5:E:140:THR:CG2	5:E:141:LYS:N	2.77	0.46
10:J:48:ILE:N	10:J:48:ILE:CD1	2.78	0.46
10:J:92:VAL:CG1	10:J:93:GLU:N	2.78	0.46
13:M:95:LEU:O	13:M:109:ARG:NH1	2.48	0.46
13:M:22:TYR:CE2	13:M:69:LEU:HD13	2.50	0.46
13:M:96:PRO:HB2	13:M:100:GLN:OE1	2.14	0.46
20:T:89:GLY:O	20:T:90:ALA:CB	2.63	0.46
23:Z:41:C:H2'	23:Z:42:C:C5'	2.45	0.46
1:A:688:G:H5'	11:K:37:VAL:HG12	1.97	0.46
1:A:707:C:O2'	1:A:708:C:H5'	2.15	0.46
1:A:997:U:C2'	1:A:998:G:H5"	2.45	0.46
2:B:76:ARG:HB3	2:B:88:ASN:ND2	2.31	0.46
9:I:125:SER:C	9:I:127:ARG:N	2.68	0.46
9:I:125:SER:O	9:I:127:ARG:N	2.48	0.46
10:J:85:THR:C	10:J:86:LEU:HD23	2.34	0.46
9:I:110:ARG:HD2	14:N:60:TRP:O	2.15	0.46
16:P:19:ILE:HG22	16:P:36:ILE:HG13	1.97	0.46
17:Q:58:ILE:HD13	17:Q:72:VAL:HA	1.96	0.46
19:S:14:LEU:CD2	19:S:14:LEU:H	2.28	0.46
19:S:29:LEU:HA	19:S:47:THR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:16:ARG:HH11	20:T:16:ARG:HG2	1.80	0.46
20:T:80:LYS:O	20:T:84:LEU:HB2	2.16	0.46
1:A:1249:C:H2'	1:A:1250:A:H5"	1.96	0.46
1:A:1483:A:H2'	1:A:1484:C:O4'	2.15	0.46
2:B:174:LEU:C	2:B:176:ILE:H	2.18	0.46
3:C:136:ALA:O	3:C:139:ARG:HG2	2.16	0.46
5:E:11:ARG:CD	5:E:22:PHE:CD2	2.94	0.46
5:E:47:VAL:HB	5:E:48:PRO:CD	2.45	0.46
5:E:74:HIS:CE1	5:E:138:LEU:HD23	2.50	0.46
8:H:107:LEU:N	8:H:107:LEU:HD23	2.29	0.46
18:R:2:SER:H	18:R:4:LYS:HZ1	1.61	0.46
1:A:1062:U:H2'	1:A:1063:C:C6	2.51	0.46
1:A:106:C:O2	1:A:379:C:H4'	2.15	0.46
1:A:1124:G:N2	1:A:1127:G:N2	2.64	0.46
1:A:1329:A:O2'	1:A:1330:U:H5'	2.15	0.46
1:A:189:G:H1	1:A:189(K):U:H3	1.63	0.46
1:A:361:G:C3'	1:A:362:G:H5"	2.43	0.46
1:A:422:C:C2'	1:A:422:C:O2	2.64	0.46
1:A:436:C:H2'	1:A:437:U:C6	2.50	0.46
1:A:715:A:H2'	1:A:716:A:C8	2.50	0.46
1:A:899:C:H2'	1:A:900:A:C8	2.50	0.46
3:C:69:VAL:HG12	3:C:71:LYS:N	2.21	0.46
4:D:172:TRP:O	4:D:185:LEU:HB2	2.14	0.46
4:D:30:CYS:O	4:D:31:ALA:HB3	2.16	0.46
5:E:135:LEU:C	5:E:137:GLN:N	2.67	0.46
5:E:13:ALA:HB2	5:E:22:PHE:CD2	2.51	0.46
5:E:3:GLU:O	5:E:30:VAL:HA	2.15	0.46
10:J:67:ASN:O	10:J:68:ARG:HD3	2.15	0.46
12:L:37:ARG:HB3	12:L:37:ARG:HH11	1.78	0.46
14:N:23:CYS:N	14:N:32:VAL:CG1	2.78	0.46
17:Q:73:LEU:C	17:Q:73:LEU:CD2	2.84	0.46
20:T:4:SER:HA	20:T:6:LEU:HD12	1.97	0.46
1:A:1030:C:H6	1:A:1030:C:H5'	1.81	0.46
1:A:17:U:O2'	1:A:1079:G:H1'	2.15	0.46
1:A:952:U:O2'	1:A:953:G:H5'	2.15	0.46
2:B:155:ALA:HB1	2:B:179:ILE:HD11	1.98	0.46
3:C:67:VAL:HG12	3:C:69:VAL:HG23	1.97	0.46
4:D:175:LEU:HA	4:D:182:GLY:HA2	1.98	0.46
5:E:148:ARG:CZ	8:H:44:PHE:CZ	2.98	0.46
2:B:172:ARG:NH2	8:H:74:PRO:HG3	2.31	0.46
10:J:57:SER:O	10:J:58:ARG:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:74:ASN:C	10:J:76:ASN:H	2.18	0.46
13:M:24:ILE:HG13	13:M:65:LEU:HD23	1.97	0.46
15:O:61:GLN:HA	15:O:61:GLN:NE2	2.31	0.46
17:Q:8:VAL:HG21	17:Q:83:LEU:CD1	2.45	0.46
18:R:28:PHE:O	18:R:36:LEU:HG	2.15	0.46
19:S:27:LYS:HD3	19:S:28:ARG:H	1.80	0.46
1:A:1140:C:C2'	1:A:1141:C:H5"	2.45	0.46
1:A:1288:A:H2'	1:A:1289:A:H8	1.81	0.46
1:A:1472:U:C2'	1:A:1473:A:O4'	2.60	0.46
2:B:92:LEU:O	2:B:95:MET:HG3	2.16	0.46
3:C:27:GLN:O	3:C:31:LEU:HG	2.16	0.46
4:D:121:ARG:C	4:D:123:GLY:H	2.19	0.46
4:D:127:VAL:O	4:D:129:GLY:N	2.49	0.46
4:D:24:ARG:C	4:D:26:TYR:N	2.69	0.46
5:E:124:PRO:O	5:E:125:ILE:C	2.54	0.46
1:A:933:G:OP2	7:G:2:ARG:HB3	2.14	0.46
9:I:8:ARG:HD3	9:I:13:VAL:HG22	1.98	0.46
9:I:80:ILE:HG22	9:I:80:ILE:O	2.16	0.46
12:L:49:ARG:N	12:L:49:ARG:HD2	2.30	0.46
12:L:6:LEU:HD23	12:L:6:LEU:HA	1.78	0.46
13:M:12:LYS:HE3	13:M:20:TYR:OH	2.15	0.46
17:Q:89:ILE:H	17:Q:89:ILE:HG13	1.55	0.46
17:Q:94:TYR:HD1	17:Q:94:TYR:H	1.59	0.46
18:R:68:GLU:OE1	18:R:68:GLU:HA	2.15	0.46
20:T:6:LEU:HD12	20:T:6:LEU:H	1.81	0.46
1:A:1333:A:H2'	1:A:1334:G:O4'	2.16	0.46
1:A:1475:G:C3'	1:A:1476:G:H5"	2.45	0.46
1:A:408:A:H5'	4:D:115:GLN:HB2	1.98	0.46
1:A:992:U:O4'	1:A:992:U:OP2	2.33	0.46
2:B:22:PHE:HD2	2:B:26:ILE:HD11	1.81	0.46
7:G:147:ASN:C	7:G:149:ALA:H	2.18	0.46
7:G:51:GLU:O	7:G:52:LYS:C	2.54	0.46
13:M:99:GLY:O	13:M:100:GLN:HG3	2.15	0.46
19:S:66:VAL:O	19:S:68:HIS:N	2.48	0.46
1:A:1314:C:C5	19:S:5:LYS:HE2	2.51	0.46
1:A:1444:C:H2'	1:A:1445:C:H6	1.81	0.46
1:A:769:G:H4'	1:A:1513:A:H4'	1.98	0.46
1:A:362:G:C8	1:A:362:G:H3'	2.51	0.46
1:A:689:C:H2'	1:A:690:G:O4'	2.15	0.46
1:A:976:G:C8	1:A:1358:U:C2	3.04	0.46
2:B:13:HIS:O	2:B:33:ILE:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:TRP:CH2	2:B:170:GLU:CD	2.89	0.46
2:B:4:LEU:HD23	2:B:42:MET:CE	2.46	0.46
11:K:86:ARG:HG2	11:K:86:ARG:NH1	2.31	0.46
12:L:39:VAL:HG12	12:L:40:THR:N	2.30	0.46
17:Q:58:ILE:CG2	17:Q:70:PHE:CD1	2.99	0.46
18:R:59:ARG:HA	18:R:64:LEU:O	2.16	0.46
1:A:1154:G:O2'	1:A:1155:G:H5'	2.15	0.46
1:A:1315:U:H2'	1:A:1316:G:O4'	2.16	0.46
1:A:1328:C:O2'	1:A:1329:A:H5'	2.16	0.46
1:A:1516:G:H2'	1:A:1518:A:OP2	2.15	0.46
1:A:433:C:H2'	1:A:434:U:C6	2.51	0.46
2:B:194:ILE:CG2	2:B:195:ILE:H	2.29	0.46
5:E:133:GLU:O	5:E:137:GLN:HB2	2.16	0.46
10:J:77:ARG:C	10:J:79:THR:H	2.19	0.46
10:J:17:SER:OG	10:J:89:PRO:HB3	2.15	0.46
1:A:130:A:C8	17:Q:62:ARG:HG3	2.50	0.46
20:T:46:LEU:O	20:T:50:ARG:HD2	2.15	0.46
1:A:1001:A:N1	1:A:1002:G:O6	2.49	0.46
1:A:106:C:HO2'	1:A:107:G:H5'	1.81	0.46
1:A:1111:A:H2'	1:A:1112:C:H6	1.80	0.46
2:B:22:PHE:HD1	2:B:188:PRO:HG3	1.81	0.46
9:I:7:GLY:HA2	9:I:78:LEU:HB3	1.97	0.46
10:J:61:PHE:HE1	14:N:57:LYS:HG2	1.79	0.46
12:L:100:VAL:O	12:L:101:TYR:HB2	2.16	0.46
19:S:19:LEU:HD12	19:S:20:GLU:HG2	1.96	0.46
1:A:1057:G:O2'	1:A:1058:G:H5'	2.17	0.45
1:A:1054:C:N4	1:A:1196:U:H5	2.15	0.45
1:A:1014:A:N3	1:A:1219:U:H1'	2.31	0.45
1:A:20:U:C2'	1:A:21:G:H5'	2.47	0.45
1:A:262:A:C6	1:A:263:A:C6	3.03	0.45
26:A:2800:RPO:O1'	26:A:2800:RPO:H1	2.16	0.45
1:A:393:A:O2'	1:A:394:G:H5'	2.16	0.45
1:A:65:U:H5"	1:A:65:U:H6	1.82	0.45
1:A:720:C:H2'	1:A:721:G:C8	2.51	0.45
1:A:731:G:O2'	1:A:732:C:H5'	2.16	0.45
2:B:102:ILE:O	2:B:102:ILE:HG22	2.15	0.45
2:B:108:ARG:NH2	2:B:112:LEU:CG	2.79	0.45
3:C:133:ILE:HG21	3:C:166:TRP:O	2.16	0.45
4:D:103:VAL:HG11	4:D:145:ILE:CD1	2.45	0.45
7:G:145:GLU:C	7:G:147:ASN:H	2.19	0.45
13:M:107:ARG:HD3	13:M:113:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:34:GLU:O	13:M:37:GLY:N	2.45	0.45
13:M:66:GLU:O	13:M:68:GLU:N	2.48	0.45
1:A:582:U:OP1	15:O:63:ARG:NH1	2.49	0.45
1:A:1041:A:H2'	1:A:1042:G:H8	1.81	0.45
1:A:1476:G:H2'	1:A:1477:C:H5'	1.99	0.45
1:A:1494:G:O2'	1:A:1495:U:H5'	2.16	0.45
1:A:955:U:O2'	1:A:956:U:H5'	2.16	0.45
3:C:5:HIS:HD2	3:C:7:ILE:H	1.64	0.45
4:D:198:ASN:C	4:D:198:ASN:ND2	2.69	0.45
6:F:37:VAL:HA	6:F:65:VAL:HG12	1.98	0.45
7:G:107:ALA:O	7:G:110:ARG:HB2	2.16	0.45
7:G:91:SER:O	7:G:95:GLN:HG2	2.16	0.45
17:Q:23:GLU:OE2	17:Q:36:LYS:HD3	2.15	0.45
21:V:5:ARG:HG2	21:V:14:ARG:HH12	1.76	0.45
1:A:1166:G:H3'	1:A:1168:A:C5'	2.46	0.45
1:A:1404:C:H2'	1:A:1405:G:C8	2.51	0.45
1:A:356:A:H1'	1:A:368:U:O2'	2.16	0.45
1:A:458:C:H2'	1:A:460:G:O4'	2.17	0.45
2:B:120:GLU:HA	2:B:123:GLU:HB3	1.98	0.45
4:D:50:PRO:HB2	4:D:55:VAL:CG2	2.46	0.45
6:F:93:SER:C	6:F:94:GLN:HG3	2.36	0.45
8:H:31:PHE:O	8:H:35:ILE:HG12	2.16	0.45
9:I:85:VAL:O	9:I:86:GLN:C	2.53	0.45
10:J:37:PRO:O	10:J:67:ASN:O	2.33	0.45
11:K:23:THR:HG22	11:K:29:PRO:HA	1.98	0.45
11:K:63:MET:O	11:K:66:GLY:N	2.49	0.45
17:Q:73:LEU:C	17:Q:73:LEU:HD23	2.37	0.45
19:S:52:ASN:HD21	19:S:55:GLN:HB2	1.80	0.45
1:A:1023:G:H2'	1:A:1023:G:N3	2.31	0.45
1:A:200:G:H2'	1:A:201:C:O4'	2.16	0.45
1:A:344:A:HO2'	1:A:345:C:P	2.40	0.45
3:C:73:GLY:O	3:C:75:VAL:N	2.49	0.45
5:E:98:ALA:HB2	5:E:116:THR:OG1	2.17	0.45
6:F:15:ASP:H	6:F:18:GLN:HE21	1.64	0.45
7:G:5:ARG:O	7:G:6:ALA:O	2.35	0.45
9:I:88:ASN:O	9:I:91:TYR:HB2	2.17	0.45
11:K:13:ALA:CB	11:K:81:ARG:HB2	2.47	0.45
1:A:1442(A):G:H5"	1:A:1442(B):A:O5'	2.17	0.45
1:A:328:C:O2	1:A:328:C:H2'	2.16	0.45
1:A:485:G:O2'	1:A:486:U:P	2.74	0.45
1:A:928:G:O2'	1:A:929:G:H5'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:PHE:HD1	2:B:179:ILE:HB	1.81	0.45
2:B:17:ARG:HD3	2:B:18:TRP:N	2.31	0.45
3:C:75:VAL:HG11	3:C:102:VAL:CG2	2.47	0.45
3:C:147:GLY:HA2	3:C:170:GLY:HA3	1.98	0.45
3:C:171:ARG:NH1	3:C:171:ARG:HB3	2.31	0.45
4:D:208:ARG:HB3	4:D:208:ARG:CZ	2.44	0.45
4:D:69:ILE:HD11	4:D:99:ARG:CD	2.46	0.45
5:E:147:LEU:HD23	8:H:79:VAL:HG22	1.96	0.45
6:F:82:ARG:HB2	6:F:85:VAL:CG2	2.47	0.45
8:H:86:ILE:HG21	8:H:133:LEU:CD2	2.23	0.45
12:L:23:LEU:HG	12:L:24:LYS:H	1.81	0.45
15:O:81:ILE:O	15:O:85:GLY:N	2.46	0.45
1:A:1090:U:H2'	1:A:1091:U:C6	2.51	0.45
1:A:431:A:O2'	1:A:432:A:H5'	2.16	0.45
4:D:9:ARG:HG2	4:D:10:LEU:N	2.32	0.45
14:N:43:LEU:HD12	14:N:43:LEU:O	2.16	0.45
20:T:83:GLN:O	20:T:86:GLU:HG2	2.16	0.45
21:V:5:ARG:CG	21:V:14:ARG:NH1	2.76	0.45
1:A:394:G:H2'	1:A:395:C:C6	2.52	0.45
1:A:403:C:H6	1:A:403:C:H5'	1.82	0.45
1:A:579:G:O2'	15:O:53:ARG:NE	2.48	0.45
1:A:811:C:O2'	1:A:901:A:N1	2.46	0.45
3:C:24:GLY:O	3:C:26:LYS:N	2.49	0.45
3:C:78:ARG:HE	3:C:81:GLU:HB3	1.79	0.45
8:H:82:HIS:CD2	8:H:83:ILE:N	2.85	0.45
19:S:50:VAL:CG2	19:S:70:LEU:HD22	2.47	0.45
1:A:194:C:O2'	20:T:61:LYS:HD3	2.17	0.45
1:A:1056:U:O2'	1:A:1057:G:H5'	2.16	0.45
1:A:1360:A:O2'	1:A:1361:G:H5'	2.17	0.45
1:A:403:C:H2'	1:A:404:U:H6	1.82	0.45
1:A:520:A:N1	1:A:536:C:H1'	2.32	0.45
1:A:50:A:H3'	1:A:52:G:C8	2.52	0.45
1:A:738:C:OP2	6:F:92:LYS:NZ	2.43	0.45
1:A:858:G:C8	1:A:858:G:C4'	3.00	0.45
1:A:957:U:C3'	1:A:958:A:C5'	2.95	0.45
1:A:957:U:N3	1:A:960:U:H5"	2.25	0.45
1:A:967:C:H4'	9:I:127:ARG:NE	2.31	0.45
1:A:972:C:P	10:J:55:LYS:HD3	2.56	0.45
2:B:126:LYS:HA	2:B:129:GLN:CB	2.41	0.45
4:D:125:ILE:HG22	4:D:126:THR:N	2.30	0.45
5:E:74:HIS:HD2	8:H:107:LEU:HD12	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:47:LEU:HB3	13:M:52:VAL:HG23	1.98	0.45
6:F:91:VAL:CG1	18:R:57:ARG:NH2	2.80	0.45
19:S:15:LEU:C	19:S:17:LYS:H	2.20	0.45
20:T:16:ARG:NH1	20:T:16:ARG:HG2	2.31	0.45
20:T:48:ILE:HD13	20:T:51:LYS:HD2	1.99	0.45
1:A:1111:A:N1	3:C:176:THR:HG22	2.32	0.45
1:A:1278:U:O2'	1:A:1279:A:OP1	2.34	0.45
1:A:1287:A:H2'	1:A:1288:A:C8	2.52	0.45
1:A:1479:C:H2'	1:A:1480:G:C5'	2.32	0.45
1:A:234:C:H2'	1:A:235:C:H6	1.82	0.45
1:A:261:U:O2	1:A:263:A:C8	2.70	0.45
1:A:567:G:H2'	1:A:568:G:O4'	2.17	0.45
1:A:778:G:C2'	1:A:779:C:H5'	2.46	0.45
2:B:158:VAL:HG22	2:B:180:ALA:HB2	1.99	0.45
2:B:213:VAL:HA	2:B:216:ILE:HG12	1.99	0.45
2:B:21:LYS:HB3	2:B:188:PRO:HD2	1.98	0.45
2:B:21:LYS:HD2	2:B:187:ASP:OD2	2.17	0.45
3:C:83:ILE:O	3:C:83:ILE:HG12	2.16	0.45
4:D:181:LYS:NZ	4:D:181:LYS:HB3	2.32	0.45
4:D:29:LYS:O	4:D:31:ALA:N	2.50	0.45
2:B:172:ARG:NH2	8:H:68:ARG:HH22	2.13	0.45
11:K:81:ARG:CD	18:R:73:LYS:HZ3	2.26	0.45
1:A:1414:U:H2'	1:A:1415:G:H8	1.81	0.45
1:A:555:C:H2'	1:A:556:C:C6	2.52	0.45
1:A:780:A:C2	1:A:801:U:C5	3.05	0.45
1:A:883:C:O2'	1:A:884:U:H5'	2.17	0.45
2:B:19:ASN:C	2:B:19:ASN:ND2	2.70	0.45
8:H:65:TYR:CD1	8:H:65:TYR:N	2.85	0.45
10:J:51:PRO:HA	14:N:41:ILE:CD1	2.47	0.45
15:O:5:GLU:HG2	15:O:6:GLU:H	1.81	0.45
1:A:135:C:C2	16:P:1:MET:HB2	2.45	0.45
1:A:1230:C:H2'	1:A:1231:G:H8	1.82	0.44
1:A:147:G:H8	1:A:147:G:H5'	1.82	0.44
1:A:598:U:H4'	8:H:94:TYR:CG	2.52	0.44
2:B:10:HIS:CG	2:B:11:PHE:N	2.81	0.44
2:B:76:ARG:CZ	2:B:76:ARG:HB2	2.47	0.44
3:C:46:LEU:HD12	3:C:46:LEU:H	1.82	0.44
4:D:27:SER:O	4:D:29:LYS:N	2.50	0.44
6:F:21:LEU:O	6:F:25:ILE:HD12	2.17	0.44
8:H:91:ARG:HH11	17:Q:32:GLY:HA3	1.82	0.44
17:Q:21:LEU:HD11	17:Q:38:SER:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:14:LEU:O	19:S:18:VAL:N	2.50	0.44
1:A:433:C:H6	1:A:433:C:O5'	1.99	0.44
1:A:702:A:O2'	1:A:703:G:OP1	2.35	0.44
2:B:49:PHE:CE2	2:B:212:ALA:HA	2.51	0.44
2:B:3:GLU:OE1	2:B:4:LEU:N	2.46	0.44
3:C:118:ARG:HG2	3:C:139:ARG:HH12	1.83	0.44
1:A:437:U:C5'	4:D:154:LEU:HD21	2.47	0.44
6:F:100:ASN:OD1	6:F:100:ASN:O	2.35	0.44
10:J:73:ILE:O	10:J:74:ASN:CB	2.63	0.44
11:K:115:PHE:O	11:K:116:ARG:CB	2.65	0.44
18:R:22:VAL:HG22	18:R:63:LEU:HB3	1.99	0.44
19:S:27:LYS:C	19:S:28:ARG:HG3	2.38	0.44
19:S:44:VAL:HA	19:S:61:ILE:CD1	2.46	0.44
19:S:71:GLY:C	19:S:73:PHE:H	2.20	0.44
20:T:67:LYS:CG	20:T:68:ASN:H	2.26	0.44
20:T:82:ARG:HB2	20:T:97:LEU:HD13	1.99	0.44
1:A:1040:U:H2'	1:A:1041:A:C8	2.52	0.44
1:A:1055:A:N6	1:A:1206:G:C5	2.85	0.44
1:A:1058:G:C6	1:A:1059:C:N3	2.85	0.44
1:A:1256:A:O3'	1:A:1257:U:C4'	2.66	0.44
1:A:1347:G:H22	1:A:1373:G:H2'	1.82	0.44
1:A:1372:U:H2'	1:A:1373:G:O4'	2.17	0.44
1:A:263:A:OP2	20:T:72:ARG:NH1	2.51	0.44
1:A:620:C:H2'	1:A:621:A:O4'	2.16	0.44
1:A:865:A:H1'	1:A:918:A:O2'	2.17	0.44
1:A:997:U:H2'	1:A:998:G:O4'	2.18	0.44
2:B:130:VAL:HA	2:B:133:LYS:HE2	1.99	0.44
3:C:166:TRP:HB3	3:C:167:ALA:H	1.41	0.44
4:D:195:LEU:HD23	4:D:196:PRO:HD2	1.99	0.44
4:D:61:GLN:CA	4:D:61:GLN:HE21	2.22	0.44
5:E:77:GLU:HG2	5:E:86:VAL:HG13	1.99	0.44
6:F:91:VAL:HG13	18:R:57:ARG:NH2	2.32	0.44
8:H:121:ASP:HB2	8:H:125:ARG:HH21	1.83	0.44
12:L:57:THR:C	12:L:59:GLY:N	2.70	0.44
13:M:97:VAL:HG12	13:M:97:VAL:O	2.17	0.44
15:O:16:ARG:NH1	15:O:76:ARG:NH1	2.65	0.44
17:Q:5:LEU:N	17:Q:58:ILE:O	2.47	0.44
20:T:87:ALA:O	20:T:88:ALA:HB3	2.18	0.44
21:V:12:ILE:HD13	21:V:21:ARG:CZ	2.47	0.44
1:A:1258:G:O2'	1:A:1259:C:H5'	2.17	0.44
1:A:167:G:H2'	1:A:168:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:G:OP2	17:Q:99:LYS:HG3	2.18	0.44
1:A:591:U:H2'	1:A:592:G:C8	2.52	0.44
4:D:35:ARG:HD2	4:D:37:TYR:CE1	2.52	0.44
4:D:99:ARG:NH1	4:D:136:SER:HA	2.32	0.44
5:E:24:PHE:CD1	5:E:24:PHE:N	2.84	0.44
7:G:19:ASP:OD2	7:G:21:LEU:HB3	2.17	0.44
10:J:23:GLU:O	10:J:25:ALA:N	2.50	0.44
11:K:4:VAL:O	11:K:5:ALA:HB3	2.18	0.44
15:O:53:ARG:O	15:O:57:MET:HG3	2.17	0.44
1:A:1036:G:O2'	1:A:1037:C:H5'	2.17	0.44
1:A:109:A:H2'	1:A:326:G:N2	2.33	0.44
1:A:1102:A:C6	1:A:1103:C:N4	2.85	0.44
1:A:126:G:H4'	1:A:634:C:O2	2.16	0.44
1:A:1460:A:H2'	1:A:1461:G:O4'	2.17	0.44
1:A:1494:G:O6	26:A:2800:RPO:HBT	2.17	0.44
1:A:370:C:H2'	1:A:371:G:H8	1.82	0.44
1:A:427:U:C4	1:A:428:G:C6	3.05	0.44
3:C:194:VAL:O	3:C:195:LEU:HD22	2.17	0.44
3:C:82:ARG:C	3:C:84:ARG:N	2.71	0.44
3:C:90:LEU:HD13	3:C:98:VAL:CG1	2.47	0.44
4:D:148:ALA:HB3	4:D:151:SER:CB	2.45	0.44
4:D:12:ARG:NH1	4:D:37:TYR:O	2.51	0.44
5:E:11:ARG:O	5:E:12:THR:O	2.35	0.44
10:J:6:LEU:HB3	10:J:14:LEU:HD22	1.98	0.44
10:J:1:LYS:CG	10:J:73:ILE:HG23	2.41	0.44
1:A:1018:C:O5'	1:A:1018:C:H6	2.00	0.44
1:A:1360:A:H8	1:A:1360:A:OP1	2.00	0.44
1:A:159:G:N2	1:A:161:A:H3'	2.28	0.44
1:A:191:G:H1'	20:T:98:SER:HA	2.00	0.44
2:B:213:VAL:HA	2:B:216:ILE:CG1	2.47	0.44
3:C:96:LYS:O	3:C:97:ASN:C	2.55	0.44
4:D:152:ARG:HG2	4:D:180:MET:CE	2.48	0.44
4:D:51:SER:O	4:D:52:ASP:C	2.56	0.44
5:E:85:ILE:HD13	5:E:86:VAL:H	1.82	0.44
6:F:33:TYR:HD2	6:F:75:LEU:HD23	1.81	0.44
7:G:15:LEU:N	7:G:15:LEU:HD22	2.33	0.44
9:I:113:TYR:CE2	10:J:57:SER:O	2.70	0.44
13:M:52:VAL:HG12	13:M:52:VAL:O	2.16	0.44
13:M:9:PRO:O	13:M:10:ARG:HB2	2.17	0.44
21:V:23:ARG:O	21:V:24:LYS:CB	2.65	0.44
1:A:1067:A:H4'	1:A:1068:G:OP1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1176:A:H2'	1:A:1177:G:O4'	2.18	0.44
1:A:1354:C:O2'	1:A:1355:G:H5'	2.17	0.44
1:A:1496:C:H2'	1:A:1497:G:O4'	2.18	0.44
1:A:1514:C:H2'	1:A:1515:C:H6	1.81	0.44
1:A:191:G:C4	20:T:98:SER:HB3	2.52	0.44
1:A:810:C:O2'	1:A:811:C:H5'	2.17	0.44
1:A:860:A:H2'	1:A:861:G:O4'	2.18	0.44
2:B:207:LEU:HD23	2:B:207:LEU:C	2.38	0.44
2:B:92:LEU:HD23	2:B:92:LEU:H	1.83	0.44
7:G:74:VAL:HB	7:G:85:GLN:HB3	2.00	0.44
7:G:76:SER:HA	7:G:84:TYR:O	2.18	0.44
10:J:12:LYS:HB3	10:J:12:LYS:NZ	2.32	0.44
10:J:19:GLN:O	10:J:22:VAL:HG12	2.18	0.44
1:A:881:G:P	12:L:8:ARG:NH2	2.90	0.44
14:N:11:ARG:C	14:N:13:PRO:HD3	2.38	0.44
17:Q:26:PHE:CE1	17:Q:35:ILE:HD11	2.52	0.44
1:A:1405:G:O4'	1:A:1519:A:H4'	2.17	0.44
1:A:1504:G:OP1	1:A:1507:A:H4'	2.17	0.44
1:A:186:C:H2'	1:A:187:C:H6	1.82	0.44
1:A:342:C:H5'	1:A:343:U:OP2	2.18	0.44
1:A:362:G:C8	1:A:362:G:C3'	3.01	0.44
1:A:575:G:H4'	1:A:576:G:C5'	2.47	0.44
2:B:17:ARG:HH12	2:B:185:ASP:CB	2.30	0.44
2:B:98:ASN:O	2:B:102:ILE:HG12	2.18	0.44
3:C:127:PHE:N	3:C:127:PHE:CD1	2.85	0.44
3:C:78:ARG:NE	3:C:81:GLU:CB	2.75	0.44
5:E:14:ARG:HH11	5:E:21:ARG:HB2	1.83	0.44
6:F:46:ARG:HB2	6:F:60:PHE:HE1	1.83	0.44
5:E:147:LEU:CD2	8:H:79:VAL:HA	2.46	0.44
9:I:115:LYS:HE3	9:I:121:ALA:HB2	1.99	0.44
10:J:23:GLU:C	10:J:25:ALA:N	2.71	0.44
10:J:4:ILE:HG22	10:J:96:ILE:HA	2.00	0.44
13:M:9:PRO:HB3	13:M:17:ALA:O	2.18	0.44
16:P:59:TRP:HB3	16:P:64:ALA:CB	2.44	0.44
17:Q:44:HIS:NE2	17:Q:46:PRO:HG3	2.33	0.44
1:A:721:G:OP2	18:R:48:GLN:HG2	2.18	0.44
20:T:36:LEU:O	20:T:39:GLU:HB2	2.18	0.44
1:A:1069:C:O2'	1:A:1192:C:H1'	2.18	0.44
1:A:153:C:C2'	1:A:154:C:H5'	2.48	0.44
1:A:36:C:O2'	1:A:37:U:H5'	2.17	0.44
1:A:767:A:H2'	1:A:768:A:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:LEU:O	2:B:39:GLN:C	2.55	0.44
5:E:85:ILE:HG13	5:E:131:THR:CG2	2.45	0.44
5:E:97:ILE:O	5:E:97:ILE:HG22	2.17	0.44
8:H:116:LYS:CD	8:H:127:LEU:HD12	2.41	0.44
9:I:91:TYR:C	9:I:93:ALA:N	2.71	0.44
11:K:59:ALA:CB	11:K:93:LEU:HD12	2.41	0.44
1:A:264:U:O2'	17:Q:63:PRO:HB2	2.17	0.44
1:A:1014:A:H4'	19:S:13:HIS:ND1	2.33	0.43
1:A:255:G:O6	1:A:266:G:O6	2.35	0.43
1:A:344:A:H5"	1:A:345:C:C5	2.49	0.43
1:A:370:C:O2'	1:A:371:G:H5'	2.18	0.43
1:A:386:C:H2'	1:A:387:U:C5'	2.47	0.43
1:A:457:C:H42	1:A:474:G:H1	1.64	0.43
1:A:552:U:O2'	1:A:553:A:H5'	2.18	0.43
1:A:631:G:H2'	1:A:632:A:C8	2.53	0.43
1:A:746:A:C2'	1:A:747:C:H5'	2.48	0.43
1:A:895:G:H2'	1:A:896:C:H6	1.82	0.43
1:A:961:U:C2'	1:A:962:C:H5'	2.48	0.43
2:B:11:PHE:C	2:B:11:PHE:CD1	2.91	0.43
2:B:73:ASP:HA	2:B:76:ARG:HG3	1.99	0.43
4:D:3:TYR:CE2	4:D:10:LEU:HD11	2.53	0.43
4:D:23:GLU:HA	4:D:23:GLU:OE1	2.18	0.43
4:D:87:VAL:O	4:D:87:VAL:HG12	2.17	0.43
7:G:119:ILE:N	7:G:119:ILE:HD12	2.32	0.43
8:H:17:THR:HB	8:H:78:GLN:OE1	2.18	0.43
9:I:52:VAL:HG21	9:I:84:LEU:HD21	1.99	0.43
13:M:76:ASN:O	13:M:79:ARG:HB3	2.17	0.43
15:O:13:GLU:HG3	15:O:14:PHE:CD1	2.54	0.43
16:P:51:VAL:O	16:P:53:VAL:N	2.50	0.43
17:Q:23:GLU:CD	17:Q:36:LYS:HD3	2.38	0.43
1:A:1305:G:H4'	21:V:3:GLY:O	2.16	0.43
1:A:1152:A:H2'	1:A:1153:C:O4'	2.18	0.43
1:A:1305:G:O2'	1:A:1332:A:N6	2.50	0.43
1:A:1362:C:H6	1:A:1362:C:H5"	1.83	0.43
1:A:166:G:H2'	1:A:167:G:C8	2.51	0.43
1:A:251:G:O2'	1:A:252:U:C6	2.71	0.43
1:A:428:G:H5"	4:D:6:PRO:HB3	2.01	0.43
1:A:433:C:O2'	1:A:434:U:H5'	2.18	0.43
1:A:655:A:H2'	1:A:656:C:C6	2.52	0.43
1:A:815:A:H4'	1:A:817:C:C4	2.53	0.43
1:A:16:A:C2	1:A:920:U:O2	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:ILE:HG22	2:B:195:ILE:H	1.83	0.43
3:C:110:LEU:HD21	3:C:143:SER:O	2.17	0.43
3:C:142:GLU:O	3:C:144:GLY:N	2.47	0.43
3:C:153:SER:HB3	3:C:196:GLY:H	1.82	0.43
1:A:620:C:C6	4:D:134:LEU:HD13	2.52	0.43
4:D:157:ILE:O	4:D:161:LEU:HB2	2.18	0.43
9:I:105:ALA:O	9:I:106:ARG:C	2.56	0.43
12:L:24:LYS:HZ2	12:L:29:ARG:HH22	1.65	0.43
13:M:87:ARG:HG2	13:M:97:VAL:CG1	2.48	0.43
15:O:63:ARG:NH1	15:O:63:ARG:HG3	2.30	0.43
16:P:34:GLU:OE1	16:P:55:ARG:NH1	2.50	0.43
19:S:79:TYR:CZ	19:S:80:ARG:HB2	2.53	0.43
20:T:46:LEU:HB2	20:T:93:ILE:HB	1.99	0.43
1:A:1109:C:H5'	1:A:1109:C:H6	1.82	0.43
1:A:1297:C:O2	1:A:1297:C:H2'	2.18	0.43
1:A:1307:U:H2'	1:A:1308:U:C6	2.54	0.43
1:A:156:G:O2'	1:A:157:G:H5'	2.19	0.43
1:A:437:U:H5'	4:D:154:LEU:HD21	2.00	0.43
1:A:640:A:C2'	1:A:641:U:H5'	2.48	0.43
2:B:134:HIS:O	2:B:137:GLU:N	2.51	0.43
2:B:217:ILE:HG21	2:B:224:VAL:HG21	1.99	0.43
6:F:32:ASN:HD22	6:F:32:ASN:N	2.14	0.43
6:F:43:LEU:N	6:F:43:LEU:CD2	2.82	0.43
8:H:110:ALA:HB3	8:H:121:ASP:HB3	2.00	0.43
17:Q:85:GLU:O	17:Q:89:ILE:HG13	2.17	0.43
20:T:22:LYS:HB2	20:T:22:LYS:HE3	1.81	0.43
1:A:1038:C:C6	1:A:1039:C:H5	2.36	0.43
1:A:1179:A:O3'	9:I:102:THR:HG23	2.18	0.43
1:A:1304:G:H2'	1:A:1305:G:H1'	2.00	0.43
1:A:1347:G:C8	9:I:106:ARG:HB3	2.54	0.43
1:A:1447:A:HO2'	1:A:1452:C:P	2.40	0.43
1:A:1457:G:O2'	1:A:1458:G:H5'	2.17	0.43
1:A:197:A:N1	1:A:220:G:O2'	2.46	0.43
1:A:457:C:H2'	1:A:458:C:C6	2.47	0.43
1:A:832:C:O2'	1:A:833:U:H5'	2.19	0.43
2:B:49:PHE:HA	2:B:52:ILE:CG1	2.49	0.43
7:G:144:ALA:O	7:G:145:GLU:HB3	2.19	0.43
9:I:31:ASP:O	9:I:34:GLU:HB3	2.18	0.43
10:J:90:THR:HG23	10:J:91:GLY:N	2.33	0.43
11:K:98:ILE:O	18:R:72:ARG:N	2.51	0.43
13:M:124:ARG:HD2	13:M:125:LYS:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:22:TYR:CD2	13:M:69:LEU:HD13	2.53	0.43
18:R:64:LEU:HD22	18:R:65:PRO:HD2	2.01	0.43
23:Z:40:C:C2'	23:Z:41:C:OP1	2.67	0.43
1:A:1102:A:H2'	1:A:1103:C:C6	2.54	0.43
1:A:189(G):G:H4'	1:A:189(H):G:OP2	2.18	0.43
1:A:190:U:O2'	1:A:191:G:H5'	2.18	0.43
1:A:404:U:C2	1:A:405:U:C5	3.07	0.43
1:A:764:C:H2'	1:A:765:G:O4'	2.19	0.43
2:B:11:PHE:CB	2:B:38:LEU:HD21	2.48	0.43
3:C:12:GLY:O	3:C:13:ILE:HD13	2.18	0.43
4:D:7:VAL:HG21	4:D:114:ARG:NH1	2.33	0.43
5:E:47:VAL:N	5:E:48:PRO:HD2	2.33	0.43
7:G:147:ASN:C	7:G:149:ALA:N	2.71	0.43
8:H:103:VAL:HG21	8:H:110:ALA:HB2	2.01	0.43
14:N:53:PRO:C	14:N:55:VAL:H	2.21	0.43
15:O:55:LEU:O	15:O:59:VAL:HG23	2.19	0.43
1:A:1019:C:O2'	1:A:1020:U:H5'	2.19	0.43
1:A:999:C:H42	1:A:1042:G:H1	1.67	0.43
1:A:1099:G:C6	1:A:1100:C:N3	2.87	0.43
1:A:1230:C:O2'	13:M:125:LYS:HB3	2.19	0.43
1:A:1321:C:C3'	1:A:1322:C:H5"	2.36	0.43
1:A:407:G:H2'	1:A:408:A:H8	1.84	0.43
1:A:413:G:H2'	1:A:428:G:H22	1.81	0.43
1:A:789:U:H2'	1:A:791:G:OP2	2.19	0.43
2:B:101:THR:O	2:B:103:SER:N	2.52	0.43
2:B:82:ALA:C	2:B:84:MET:H	2.22	0.43
2:B:72:GLN:O	2:B:88:ASN:OD1	2.37	0.43
3:C:42:LEU:HD13	3:C:67:VAL:CG2	2.49	0.43
4:D:95:LEU:O	4:D:98:SER:HB2	2.19	0.43
7:G:22:VAL:HG13	7:G:42:PHE:CE2	2.54	0.43
8:H:60:ARG:NH1	8:H:60:ARG:HG3	2.30	0.43
1:A:1061:G:H1'	10:J:54:HIS:CE1	2.53	0.43
1:A:716:A:N3	11:K:107:ASN:O	2.51	0.43
18:R:10:THR:O	18:R:11:LEU:CB	2.67	0.43
19:S:3:SER:OG	19:S:4:LEU:N	2.52	0.43
20:T:93:ILE:C	20:T:95:GLY:N	2.70	0.43
1:A:1027:C:C6	1:A:1027:C:H5'	2.48	0.43
1:A:1145:C:C4'	1:A:1146:A:H5'	2.48	0.43
1:A:1429:C:H2'	1:A:1430:C:C6	2.52	0.43
1:A:35:G:H2'	1:A:36:C:H6	1.82	0.43
1:A:374:A:C6	1:A:375:U:C4	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:U:C5	1:A:381:C:C4	3.07	0.43
2:B:187:ASP:HB3	2:B:190:LEU:HD12	2.01	0.43
4:D:186:ARG:HG3	4:D:187:LEU:H	1.83	0.43
7:G:114:ARG:HB2	7:G:117:VAL:HG23	2.00	0.43
1:A:564:C:OP1	12:L:11:ARG:NE	2.51	0.43
15:O:30:LEU:N	15:O:30:LEU:HD12	2.34	0.43
15:O:52:HIS:O	15:O:55:LEU:HB3	2.18	0.43
1:A:190:U:C2	20:T:98:SER:HB2	2.53	0.43
1:A:1168:A:H3'	1:A:1169:A:H8	1.83	0.43
1:A:1281:U:H5"	1:A:1282:C:H5	1.84	0.43
1:A:1372:U:OP1	9:I:71:GLY:N	2.48	0.43
1:A:285:G:O2'	1:A:286:G:H5'	2.18	0.43
1:A:416:G:H2'	1:A:417:C:C6	2.54	0.43
3:C:124:GLU:HG2	3:C:189:ARG:O	2.18	0.43
3:C:6:PRO:HG2	3:C:183:TYR:CD1	2.54	0.43
3:C:28:TYR:OH	14:N:53:PRO:HD2	2.19	0.43
8:H:60:ARG:CG	8:H:60:ARG:HH11	2.21	0.43
12:L:25:GLY:O	12:L:26:ALA:O	2.35	0.43
12:L:81:ILE:HA	12:L:81:ILE:HD12	1.85	0.43
15:O:21:THR:O	15:O:26:VAL:HG11	2.18	0.43
21:V:13:TRP:C	21:V:15:GLY:N	2.71	0.43
1:A:1314:C:OP2	19:S:5:LYS:CD	2.67	0.43
1:A:1365:G:C6	1:A:1366:C:C4	3.07	0.43
1:A:1367:C:H5'	10:J:58:ARG:NH2	2.23	0.43
1:A:1345:U:C2	1:A:1377:A:C2	3.07	0.43
1:A:243:A:H4'	1:A:244:U:H5"	2.01	0.43
1:A:308:C:H2'	1:A:309:G:H8	1.84	0.43
1:A:410:G:OP2	4:D:24:ARG:HD2	2.18	0.43
2:B:10:HIS:O	2:B:11:PHE:CG	2.72	0.43
2:B:14:GLU:HB2	2:B:184:THR:HB	2.00	0.43
2:B:186:SER:O	2:B:188:PRO:HD3	2.18	0.43
3:C:86:LEU:O	3:C:89:GLU:HB3	2.19	0.43
4:D:106:ARG:HB3	4:D:173:LEU:HD11	2.01	0.43
4:D:152:ARG:HG3	4:D:180:MET:SD	2.59	0.43
9:I:32:PHE:CE2	9:I:46:LEU:HD11	2.54	0.43
9:I:78:LEU:HD11	9:I:82:ARG:NE	2.34	0.43
14:N:24:VAL:HG13	14:N:25:ARG:N	2.33	0.43
10:J:45:PHE:CE2	14:N:36:PHE:HE2	2.36	0.43
14:N:39:CYS:O	14:N:43:LEU:HB3	2.19	0.43
19:S:28:ARG:HH11	19:S:28:ARG:HG3	1.83	0.43
1:A:1320:C:N3	19:S:35:ARG:HD3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:40:VAL:HB	19:S:41:PRO:HD2	2.00	0.43
19:S:48:ILE:CD1	19:S:48:ILE:N	2.77	0.43
20:T:69:ALA:HA	20:T:72:ARG:NH1	2.34	0.43
1:A:1151:A:O2'	1:A:1152:A:H5"	2.19	0.43
1:A:1360:A:H2'	1:A:1361:G:O4'	2.19	0.43
1:A:388:G:OP1	1:A:388:G:H8	2.02	0.43
1:A:556:C:C2'	1:A:557:G:H5'	2.49	0.43
2:B:134:HIS:HA	2:B:137:GLU:CG	2.46	0.43
3:C:112:ALA:HB3	3:C:113:PRO:HD3	2.01	0.43
3:C:63:VAL:HG12	3:C:65:VAL:CG2	2.45	0.43
3:C:78:ARG:CD	3:C:78:ARG:O	2.63	0.43
6:F:44:GLY:O	6:F:59:TYR:HA	2.19	0.43
6:F:62:TRP:CG	6:F:63:TYR:N	2.87	0.43
9:I:4:TYR:CG	9:I:5:GLY:N	2.87	0.43
10:J:74:ASN:O	10:J:76:ASN:ND2	2.52	0.43
11:K:101:ASP:O	11:K:101:ASP:CG	2.57	0.43
13:M:83:ILE:HG13	13:M:85:CYS:H	1.84	0.43
20:T:3:LEU:O	20:T:6:LEU:CD1	2.67	0.43
1:A:1074:G:O3'	2:B:97:THR:HG22	2.18	0.42
1:A:1140:C:H2'	1:A:1141:C:C5'	2.47	0.42
1:A:1457:G:H2'	1:A:1458:G:H8	1.82	0.42
1:A:411:A:C5	1:A:429:U:C5	3.07	0.42
2:B:45:LEU:O	2:B:49:PHE:HD1	2.01	0.42
3:C:72:PRO:O	3:C:75:VAL:HB	2.19	0.42
4:D:7:VAL:HG11	4:D:20:LEU:HB3	2.00	0.42
5:E:72:ILE:HD12	5:E:138:LEU:HD11	1.99	0.42
7:G:137:LYS:C	7:G:137:LYS:HD2	2.39	0.42
10:J:10:ASP:OD1	10:J:12:LYS:N	2.45	0.42
10:J:2:ILE:HA	10:J:2:ILE:HD13	1.91	0.42
18:R:39:ARG:HH21	18:R:40:ARG:HG3	1.83	0.42
18:R:19:TYR:HA	18:R:54:THR:HG23	2.00	0.42
20:T:50:ARG:HE	20:T:93:ILE:CG2	2.25	0.42
1:A:232:G:H1'	1:A:262:A:N1	2.34	0.42
1:A:298:A:H2'	1:A:299:G:O4'	2.19	0.42
2:B:108:ARG:NH2	2:B:112:LEU:HD21	2.33	0.42
2:B:91:TRP:CH2	2:B:170:GLU:OE2	2.72	0.42
3:C:194:VAL:HG12	3:C:195:LEU:N	2.34	0.42
3:C:206:VAL:CG1	3:C:207:ILE:N	2.80	0.42
3:C:69:VAL:CG1	3:C:70:ALA:N	2.81	0.42
4:D:148:ALA:O	4:D:149:GLU:C	2.57	0.42
4:D:81:ALA:C	4:D:88:THR:HG23	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:140:THR:HG22	5:E:142:ALA:N	2.34	0.42
8:H:10:LEU:HD12	8:H:85:ARG:CG	2.49	0.42
10:J:32:VAL:HG22	10:J:72:ILE:CG2	2.49	0.42
10:J:70:VAL:HG12	10:J:71:ASP:N	2.33	0.42
13:M:58:TYR:O	13:M:62:THR:CG2	2.67	0.42
15:O:26:VAL:O	15:O:30:LEU:HD13	2.19	0.42
18:R:51:LEU:O	18:R:55:ILE:HG12	2.19	0.42
20:T:66:HIS:O	20:T:67:LYS:CB	2.67	0.42
23:Z:31:A:H2'	23:Z:32:U:C6	2.53	0.42
1:A:1008:C:O2'	1:A:1009:G:H5'	2.19	0.42
1:A:104:G:N7	20:T:7:LYS:NZ	2.57	0.42
1:A:1069:C:H2'	1:A:1070:U:H5"	2.02	0.42
1:A:1422:G:O2'	1:A:1423:G:H5'	2.18	0.42
1:A:176:C:O2'	1:A:177:C:H5'	2.19	0.42
1:A:31:G:O2'	1:A:48:C:N4	2.52	0.42
1:A:614:A:C2	1:A:627:G:C2	3.08	0.42
1:A:858:G:O5'	1:A:858:G:H8	2.02	0.42
2:B:189:ASP:O	8:H:68:ARG:NH2	2.52	0.42
2:B:45:LEU:CD2	2:B:49:PHE:HE1	2.30	0.42
4:D:16:VAL:N	4:D:32:MET:HE1	2.34	0.42
4:D:62:LYS:O	4:D:66:ILE:HG13	2.19	0.42
5:E:69:ASN:C	5:E:71:THR:H	2.22	0.42
6:F:39:LYS:NZ	6:F:64:GLN:HE21	2.17	0.42
6:F:67:MET:HB2	6:F:68:PRO:HD2	2.02	0.42
7:G:14:ASP:OD1	7:G:15:LEU:N	2.51	0.42
8:H:11:THR:HA	8:H:14:ARG:HH12	1.84	0.42
8:H:82:HIS:C	8:H:82:HIS:CD2	2.91	0.42
10:J:20:LYS:HZ1	10:J:88:LEU:H	1.67	0.42
3:C:28:TYR:HE2	10:J:9:PHE:HE2	1.66	0.42
13:M:83:ILE:C	13:M:85:CYS:H	2.22	0.42
16:P:4:ILE:HA	16:P:20:VAL:O	2.19	0.42
16:P:4:ILE:HG23	16:P:36:ILE:HD11	2.01	0.42
19:S:43:MET:O	19:S:44:VAL:C	2.58	0.42
1:A:1355:G:O2'	1:A:1356:G:H5'	2.19	0.42
1:A:189(I):G:C2'	1:A:189(J):G:H5'	2.48	0.42
1:A:314:C:O2'	1:A:315:A:H5'	2.19	0.42
1:A:370:C:H2'	1:A:371:G:C8	2.53	0.42
1:A:737:A:H2'	1:A:738:C:C6	2.55	0.42
1:A:858:G:N1	1:A:869:G:C8	2.87	0.42
3:C:130:ARG:CZ	3:C:130:ARG:HB2	2.48	0.42
3:C:69:VAL:O	3:C:105:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:10:LEU:HD12	8:H:85:ARG:HG2	2.01	0.42
9:I:79:GLY:C	9:I:81:ALA:H	2.22	0.42
14:N:21:THR:CB	14:N:32:VAL:HG21	2.50	0.42
14:N:5:LEU:C	14:N:7:GLU:N	2.72	0.42
21:V:23:ARG:O	21:V:24:LYS:CG	2.67	0.42
1:A:1055:A:H2'	1:A:1055:A:N3	2.34	0.42
1:A:949:A:C2	1:A:1233:G:N3	2.88	0.42
1:A:159:G:H1	1:A:163:C:N4	2.17	0.42
1:A:189(A):C:H2'	1:A:189(B):C:H6	1.85	0.42
1:A:28:G:O2'	1:A:296:U:OP1	2.37	0.42
1:A:427:U:OP1	4:D:12:ARG:NH2	2.51	0.42
1:A:458:C:H2'	1:A:460:G:C8	2.53	0.42
1:A:725:G:O2'	1:A:726:C:H5'	2.19	0.42
1:A:750:G:O2'	1:A:751:U:H5'	2.19	0.42
1:A:772:U:O2'	1:A:773:G:H5'	2.19	0.42
1:A:889:A:OP1	1:A:889:A:H8	2.03	0.42
3:C:133:ILE:HD11	3:C:152:VAL:HG23	2.02	0.42
3:C:65:VAL:O	3:C:65:VAL:HG12	2.19	0.42
6:F:94:GLN:HE21	18:R:17:ARG:NE	2.15	0.42
8:H:16:ALA:O	8:H:19:VAL:HG22	2.19	0.42
9:I:10:LYS:O	9:I:11:GLU:HB3	2.20	0.42
9:I:54:ALA:O	9:I:55:LEU:HB3	2.18	0.42
10:J:1:LYS:CA	10:J:73:ILE:HA	2.43	0.42
12:L:43:LYS:CB	12:L:44:PRO:CD	2.70	0.42
17:Q:67:ARG:HG3	17:Q:67:ARG:NH1	2.33	0.42
19:S:43:MET:HA	19:S:46:HIS:CD2	2.41	0.42
21:V:1:GLY:O	21:V:3:GLY:N	2.52	0.42
1:A:695:A:H2'	1:A:696:A:C8	2.54	0.42
1:A:908:A:O2'	1:A:909:A:H5'	2.20	0.42
1:A:911:U:H2'	1:A:912:C:C6	2.54	0.42
2:B:68:LYS:HB2	2:B:68:LYS:HE3	1.86	0.42
3:C:106:GLN:O	3:C:107:ASN:HB3	2.20	0.42
4:D:139:VAL:HG11	4:D:145:ILE:HD11	2.01	0.42
4:D:37:TYR:HE2	4:D:44:GLN:HG2	1.84	0.42
5:E:53:LYS:O	5:E:57:TYR:CD2	2.73	0.42
5:E:69:ASN:O	5:E:71:THR:N	2.53	0.42
6:F:12:PRO:HG3	6:F:57:GLN:O	2.18	0.42
2:B:172:ARG:NH2	8:H:68:ARG:NH2	2.68	0.42
9:I:9:ARG:O	9:I:10:LYS:C	2.57	0.42
9:I:45:ALA:HB1	9:I:76:ILE:HG21	2.00	0.42
10:J:19:GLN:OE1	10:J:19:GLN:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:44:ARG:HG2	10:J:44:ARG:NH1	2.31	0.42
12:L:45:ASN:OD1	12:L:88:ASP:OD2	2.38	0.42
13:M:22:TYR:HE2	13:M:69:LEU:HB3	1.85	0.42
14:N:33:TYR:N	14:N:38:LEU:O	2.53	0.42
18:R:4:LYS:O	18:R:5:ALA:HB3	2.20	0.42
19:S:27:LYS:CD	19:S:28:ARG:H	2.33	0.42
20:T:43:GLU:HG3	20:T:93:ILE:HG12	2.00	0.42
1:A:1041:A:H2'	1:A:1042:G:C8	2.54	0.42
1:A:1260:C:H4'	1:A:1283:G:O2'	2.19	0.42
1:A:1297:C:C2'	1:A:1297:C:O2	2.66	0.42
1:A:1491:G:C5	26:A:2800:RPO:H2	2.55	0.42
1:A:460:G:H2'	1:A:461:A:H5"	2.01	0.42
1:A:499:A:H4'	1:A:500:G:O5'	2.19	0.42
1:A:598:U:H4'	8:H:94:TYR:CD2	2.55	0.42
1:A:642:A:C5	8:H:115:SER:HA	2.54	0.42
1:A:644:G:C5	1:A:645:C:C5	3.07	0.42
1:A:7:G:H5"	1:A:298:A:O4'	2.20	0.42
3:C:163:ARG:NH2	3:C:165:GLU:OE1	2.51	0.42
9:I:115:LYS:HE2	9:I:119:ARG:O	2.20	0.42
9:I:47:GLU:N	9:I:48:PRO:CD	2.83	0.42
10:J:2:ILE:O	10:J:71:ASP:HA	2.20	0.42
10:J:30:ALA:O	10:J:32:VAL:N	2.52	0.42
13:M:18:LEU:HD11	13:M:33:LEU:HD21	2.01	0.42
13:M:87:ARG:HG2	13:M:97:VAL:HG12	2.01	0.42
1:A:1082:G:O2'	1:A:1083:U:H5'	2.19	0.42
1:A:112:G:O2'	1:A:113:G:H5'	2.19	0.42
1:A:1152:A:O2'	1:A:1153:C:H5'	2.19	0.42
1:A:1246:C:O2'	1:A:1247:U:H5'	2.20	0.42
1:A:1259:C:O5'	1:A:1259:C:H6	2.03	0.42
1:A:975:A:N6	1:A:1367:C:O4'	2.52	0.42
1:A:1379:G:N7	7:G:1:ALA:HB3	2.35	0.42
1:A:1487:G:O2'	1:A:1488:G:H5'	2.19	0.42
1:A:189(B):C:H42	1:A:189(I):G:H1	1.65	0.42
1:A:300:A:H8	1:A:300:A:O5'	2.03	0.42
1:A:429:U:H4'	1:A:430:A:O5'	2.20	0.42
1:A:518:C:H2'	1:A:530:G:N3	2.34	0.42
1:A:781:A:OP1	1:A:1523:G:H5'	2.20	0.42
1:A:975:A:C5'	1:A:976:G:O5'	2.66	0.42
2:B:223:VAL:O	2:B:223:VAL:HG23	2.19	0.42
3:C:24:GLY:C	3:C:26:LYS:H	2.23	0.42
4:D:88:THR:O	4:D:88:THR:CG2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:32:ASP:OD2	5:E:36:ARG:HB2	2.19	0.42
7:G:4:ARG:HB3	7:G:5:ARG:H	1.67	0.42
8:H:103:VAL:HG21	8:H:109:ILE:C	2.39	0.42
8:H:29:SER:OG	8:H:32:LYS:HB2	2.20	0.42
9:I:78:LEU:HD13	9:I:78:LEU:C	2.40	0.42
10:J:20:LYS:HZ2	10:J:88:LEU:N	2.18	0.42
15:O:8:GLN:O	15:O:9:LYS:C	2.58	0.42
16:P:3:LYS:O	16:P:21:VAL:HA	2.19	0.42
16:P:43:LYS:HA	16:P:48:TRP:HB3	2.00	0.42
12:L:6:LEU:HB3	17:Q:31:TYR:CE2	2.55	0.42
19:S:49:ALA:HA	19:S:57:VAL:O	2.20	0.42
19:S:44:VAL:CA	19:S:61:ILE:HD12	2.47	0.42
23:Z:41:C:C6	23:Z:41:C:OP1	2.72	0.42
1:A:1272:G:O2'	1:A:1273:G:H5'	2.20	0.42
1:A:136:C:O4'	16:P:1:MET:HG2	2.20	0.42
1:A:1390:U:H2'	1:A:1391:U:H6	1.83	0.42
1:A:1476:G:C2'	1:A:1477:C:H5'	2.50	0.42
1:A:242:C:C2'	1:A:243:A:H5'	2.49	0.42
2:B:68:LYS:NZ	2:B:160:ASP:HB2	2.35	0.42
2:B:41:THR:HG23	2:B:196:PRO:HG2	2.02	0.42
2:B:215:LEU:HD13	2:B:215:LEU:C	2.40	0.42
1:A:1103:C:H5"	2:B:92:LEU:HD13	2.02	0.42
4:D:161:LEU:HD13	4:D:180:MET:SD	2.60	0.42
4:D:59:GLU:OE1	4:D:62:LYS:HD2	2.20	0.42
5:E:101:VAL:HB	5:E:102:PRO:CD	2.42	0.42
9:I:79:GLY:C	9:I:81:ALA:N	2.72	0.42
10:J:6:LEU:HD21	10:J:94:ILE:HG12	1.99	0.42
14:N:28:ARG:HB3	14:N:39:CYS:HB3	2.01	0.42
1:A:262:A:C5'	20:T:67:LYS:HG2	2.48	0.42
20:T:9:HIS:O	20:T:10:ARG:C	2.58	0.42
1:A:1229:A:H2'	1:A:1230:C:C6	2.55	0.42
1:A:1277:C:C6	1:A:1277:C:H3'	2.54	0.42
1:A:1442(A):G:C4'	1:A:1442(B):A:O5'	2.67	0.42
1:A:260:G:H2'	1:A:261:U:C6	2.55	0.42
1:A:439:A:H2'	1:A:441:A:H5'	2.02	0.42
2:B:74:ILE:HG13	2:B:202:ILE:HG23	2.02	0.42
1:A:1056:U:C5'	3:C:162:ALA:HB2	2.49	0.42
3:C:69:VAL:O	3:C:104:GLU:HA	2.19	0.42
5:E:11:ARG:HD3	5:E:22:PHE:HB3	2.02	0.42
7:G:140:VAL:O	7:G:143:MET:HB3	2.19	0.42
7:G:154:ARG:HA	7:G:154:ARG:HD3	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:32:PHE:CE1	9:I:36:PHE:HD2	2.38	0.42
10:J:14:LEU:C	10:J:16:ALA:H	2.22	0.42
10:J:23:GLU:O	10:J:27:ARG:NH1	2.53	0.42
10:J:53:LYS:HG3	10:J:54:HIS:N	2.35	0.42
14:N:44:ARG:CG	14:N:44:ARG:NH1	2.83	0.42
16:P:74:LEU:HG	16:P:79:VAL:CG2	2.27	0.42
18:R:71:VAL:O	18:R:72:ARG:CB	2.59	0.42
1:A:1149:C:H2'	1:A:1150:U:C6	2.55	0.41
1:A:1179:A:H2'	1:A:1180:A:O4'	2.20	0.41
1:A:1410:G:H2'	1:A:1411:C:C6	2.55	0.41
1:A:188:C:O2'	1:A:189:G:H5'	2.20	0.41
1:A:255:G:H1'	17:Q:15:GLN:HE22	1.81	0.41
1:A:373:A:C2	1:A:482:A:C6	3.08	0.41
1:A:45:U:H2'	1:A:46:G:C8	2.55	0.41
1:A:983:A:N3	1:A:983:A:H3'	2.35	0.41
4:D:120:VAL:O	4:D:133:ASP:HA	2.20	0.41
4:D:189:ASP:O	4:D:190:ARG:C	2.59	0.41
5:E:16:GLN:O	5:E:17:ALA:C	2.56	0.41
1:A:824:C:H4'	8:H:1:MET:N	2.35	0.41
11:K:59:ALA:HB1	11:K:93:LEU:CD1	2.44	0.41
1:A:1202:G:N1	14:N:41:ILE:HG21	2.35	0.41
16:P:67:THR:HB	16:P:70:ALA:CB	2.50	0.41
17:Q:79:GLY:O	17:Q:81:MET:N	2.53	0.41
18:R:39:ARG:CZ	18:R:40:ARG:HG3	2.50	0.41
20:T:36:LEU:HB2	20:T:45:ALA:HB2	2.01	0.41
1:A:1101:A:H4'	1:A:1102:A:O5'	2.21	0.41
1:A:1129:C:H4'	1:A:1130:A:C8	2.53	0.41
1:A:1180:A:P	9:I:102:THR:HG23	2.60	0.41
1:A:40:C:H2'	1:A:41:G:C8	2.55	0.41
1:A:551:U:H2'	1:A:552:U:C6	2.54	0.41
1:A:612:C:O5'	1:A:612:C:H6	2.03	0.41
1:A:750:G:O2'	15:O:20:ASP:OD1	2.39	0.41
1:A:8:A:H5"	5:E:97:ILE:HG23	2.01	0.41
1:A:91:C:H2'	1:A:92:C:C6	2.55	0.41
1:A:961:U:H2'	1:A:962:C:H5'	2.02	0.41
1:A:986:A:O2'	19:S:54:LYS:HA	2.20	0.41
1:A:987:G:H1	1:A:1218:C:H42	1.66	0.41
3:C:154:GLY:HA3	3:C:163:ARG:O	2.20	0.41
4:D:208:ARG:HH11	4:D:208:ARG:CB	2.26	0.41
5:E:32:ASP:OD1	5:E:34:GLN:N	2.38	0.41
9:I:96:LYS:O	9:I:98:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:47:VAL:O	10:J:58:ARG:CA	2.64	0.41
14:N:23:CYS:N	14:N:28:ARG:O	2.52	0.41
18:R:2:SER:H	18:R:4:LYS:NZ	2.17	0.41
20:T:38:GLN:O	20:T:38:GLN:CD	2.59	0.41
20:T:61:LYS:HA	20:T:61:LYS:HD2	1.95	0.41
1:A:1182:G:O2'	1:A:1183:A:P	2.79	0.41
1:A:1229:A:C2	1:A:1230:C:C4	3.08	0.41
1:A:437:U:H2'	1:A:438:G:C5'	2.50	0.41
1:A:697:U:C2'	1:A:698:G:H5'	2.50	0.41
2:B:96:LEU:O	2:B:99:PHE:HB2	2.19	0.41
3:C:127:PHE:HD1	3:C:127:PHE:N	2.18	0.41
3:C:128:ALA:H	3:C:131:ARG:NH2	2.19	0.41
3:C:153:SER:CB	3:C:196:GLY:H	2.33	0.41
3:C:31:LEU:O	3:C:35:ASP:CB	2.59	0.41
4:D:7:VAL:C	4:D:9:ARG:N	2.73	0.41
6:F:63:TYR:HB3	6:F:64:GLN:H	1.71	0.41
8:H:97:VAL:HA	8:H:100:ILE:HG13	2.01	0.41
13:M:48:THR:HG22	13:M:49:GLU:N	2.35	0.41
16:P:28:ARG:HH11	16:P:28:ARG:CG	2.31	0.41
19:S:36:ARG:HH11	19:S:36:ARG:HG2	1.84	0.41
23:Z:41:C:O2'	23:Z:42:C:H4'	2.21	0.41
1:A:1005:A:C5	1:A:1006:C:H1'	2.56	0.41
1:A:1122:U:O2'	1:A:1123:A:H5'	2.20	0.41
1:A:1223:C:H3'	1:A:1224:G:H5"	2.03	0.41
1:A:1251:A:H4'	9:I:11:GLU:CD	2.40	0.41
1:A:1499:A:H2'	1:A:1500:A:H8	1.85	0.41
1:A:627:G:H2'	1:A:628:G:H8	1.86	0.41
1:A:653:A:OP1	8:H:56:LYS:NZ	2.44	0.41
1:A:674:G:OP1	6:F:87:ARG:NH2	2.51	0.41
2:B:51:PHE:O	2:B:55:LEU:HD23	2.20	0.41
2:B:71:ALA:HB1	2:B:205:ILE:HG21	2.02	0.41
3:C:189:ARG:CB	3:C:189:ARG:HH11	2.31	0.41
7:G:125:ASP:OD1	7:G:130:LYS:HE2	2.20	0.41
21:V:9:ARG:HB2	21:V:9:ARG:NH1	2.36	0.41
1:A:1019:C:H2'	1:A:1020:U:C5'	2.49	0.41
1:A:1027:C:H2'	1:A:1028:C:C6	2.55	0.41
1:A:1071:C:H42	1:A:1104:G:H1	1.69	0.41
1:A:1103:C:H2'	1:A:1104:G:O4'	2.19	0.41
1:A:1279:A:H5'	1:A:1280:A:OP1	2.20	0.41
1:A:1365:G:C5	1:A:1366:C:C5	3.08	0.41
1:A:162:A:H8	1:A:162:A:O5'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:C:O2'	1:A:178:C:H5'	2.21	0.41
1:A:194:C:OP1	20:T:54:SER:OG	2.37	0.41
1:A:226:G:O2'	1:A:227:G:H5'	2.19	0.41
1:A:267:C:H2'	1:A:268:C:H6	1.85	0.41
1:A:322:C:H2'	1:A:323:U:C6	2.55	0.41
1:A:392:G:C2	1:A:393:A:C4	3.08	0.41
1:A:485:G:H2'	1:A:486:U:OP2	2.20	0.41
1:A:669:U:O2'	1:A:670:G:H5'	2.20	0.41
1:A:794:A:H2'	1:A:795:C:C6	2.55	0.41
1:A:949:A:H1'	1:A:1364:U:H3	1.85	0.41
1:A:951:G:OP2	13:M:101:ARG:NH2	2.50	0.41
2:B:13:HIS:CD2	2:B:199:ASP:OD1	2.73	0.41
3:C:172:VAL:N	3:C:173:PRO:CD	2.84	0.41
3:C:187:LEU:O	3:C:188:ALA:CB	2.68	0.41
4:D:3:TYR:CD2	4:D:114:ARG:NH2	2.88	0.41
4:D:37:TYR:HD1	4:D:37:TYR:N	1.98	0.41
5:E:7:ILE:HD11	5:E:29:VAL:HG22	2.02	0.41
6:F:47:ARG:NE	6:F:47:ARG:H	2.16	0.41
1:A:1178:G:P	9:I:92:ARG:HH22	2.44	0.41
10:J:7:ARG:HG2	10:J:7:ARG:HH11	1.85	0.41
10:J:88:LEU:H	10:J:89:PRO:HD3	1.85	0.41
3:C:28:TYR:HE2	10:J:9:PHE:CE2	2.38	0.41
11:K:74:VAL:HG11	11:K:81:ARG:HD3	2.03	0.41
12:L:19:LYS:C	12:L:20:VAL:HG23	2.41	0.41
13:M:62:THR:HG23	13:M:63:TRP:CD2	2.55	0.41
14:N:40:ARG:HG3	14:N:41:ILE:N	2.35	0.41
17:Q:62:ARG:HG2	17:Q:63:PRO:CD	2.50	0.41
18:R:21:ASN:O	18:R:21:ASN:ND2	2.53	0.41
18:R:56:LYS:O	18:R:60:ILE:HG12	2.20	0.41
1:A:1182:G:O2'	1:A:1183:A:OP2	2.30	0.41
1:A:1281:U:H5"	1:A:1282:C:C5	2.56	0.41
1:A:452:A:O3'	16:P:72:ARG:HD2	2.20	0.41
1:A:531:U:H4'	1:A:532:A:O5'	2.19	0.41
1:A:784:C:H2'	1:A:785:G:O5'	2.20	0.41
1:A:924:C:H5'	1:A:1399:C:OP2	2.21	0.41
3:C:130:ARG:NH1	3:C:130:ARG:CB	2.75	0.41
5:E:14:ARG:NH1	5:E:21:ARG:HB2	2.36	0.41
9:I:8:ARG:HG3	9:I:13:VAL:HG13	2.01	0.41
9:I:99:GLY:C	9:I:101:LEU:N	2.73	0.41
14:N:11:ARG:O	14:N:13:PRO:HD3	2.20	0.41
17:Q:100:ARG:HB3	17:Q:101:GLY:H	1.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:27:LYS:CG	19:S:28:ARG:N	2.82	0.41
21:V:14:ARG:HG2	21:V:14:ARG:NH1	2.35	0.41
21:V:1:GLY:C	21:V:3:GLY:N	2.73	0.41
23:Z:40:C:O5'	23:Z:40:C:H6	2.02	0.41
1:A:1001(A):G:H3'	1:A:1002:G:C8	2.52	0.41
1:A:1202:G:C6	14:N:41:ILE:HG21	2.56	0.41
2:B:6:GLU:OE1	2:B:9:VAL:CG2	2.69	0.41
4:D:150:LYS:H	4:D:150:LYS:CD	2.24	0.41
4:D:77:LEU:HB3	4:D:92:PHE:HE1	1.84	0.41
6:F:82:ARG:HB2	6:F:85:VAL:HG23	2.03	0.41
6:F:97:PHE:HB2	18:R:17:ARG:HH11	1.86	0.41
7:G:24:ALA:HA	7:G:27:ASN:HD22	1.84	0.41
8:H:68:ARG:HH11	8:H:68:ARG:HG2	1.84	0.41
10:J:40:THR:HG23	10:J:65:THR:O	2.21	0.41
11:K:100:ASP:OD2	18:R:73:LYS:CE	2.68	0.41
11:K:77:THR:CG2	11:K:81:ARG:HH21	2.19	0.41
12:L:22:ALA:C	12:L:23:LEU:O	2.59	0.41
13:M:35:LYS:CB	13:M:35:LYS:NZ	2.82	0.41
17:Q:5:LEU:HB3	17:Q:22:VAL:HG11	2.02	0.41
19:S:20:GLU:C	19:S:22:ASN:N	2.74	0.41
19:S:28:ARG:NH1	19:S:28:ARG:HG3	2.35	0.41
1:A:1058:G:OP1	3:C:198:LYS:HE3	2.21	0.41
1:A:1217:C:H2'	1:A:1218:C:O4'	2.20	0.41
1:A:222:U:H2'	1:A:223:U:C6	2.56	0.41
1:A:230:G:H2'	1:A:231:G:O4'	2.21	0.41
1:A:791:G:C6	1:A:792:A:N7	2.88	0.41
3:C:111:SER:OG	3:C:114:LEU:HG	2.20	0.41
3:C:205:GLU:O	3:C:206:VAL:O	2.37	0.41
3:C:90:LEU:CD1	3:C:98:VAL:HG22	2.51	0.41
5:E:27:LEU:HD22	5:E:39:LEU:HD21	2.02	0.41
7:G:144:ALA:C	7:G:146:ALA:N	2.72	0.41
2:B:172:ARG:NH2	8:H:74:PRO:HB3	2.29	0.41
10:J:47:VAL:O	10:J:58:ARG:C	2.59	0.41
14:N:41:ILE:O	14:N:45:GLU:HG3	2.21	0.41
14:N:25:ARG:HH21	14:N:46:LEU:HD21	1.86	0.41
1:A:1361:G:H2'	1:A:1362:C:O4'	2.21	0.41
1:A:1388:C:H2'	1:A:1389:C:C6	2.56	0.41
1:A:496:A:N3	1:A:496:A:H2'	2.36	0.41
1:A:757:U:H5"	1:A:822:C:O2	2.21	0.41
2:B:125:PRO:C	2:B:127:LYS:H	2.22	0.41
2:B:68:LYS:HZ2	2:B:160:ASP:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:THR:CG2	2:B:90:ARG:NH1	2.84	0.41
3:C:12:GLY:HA3	14:N:56:ARG:NH2	2.36	0.41
4:D:69:ILE:HG22	4:D:70:SER:O	2.20	0.41
9:I:29:GLY:O	9:I:30:GLN:O	2.38	0.41
9:I:94:LYS:C	9:I:97:PRO:HD2	2.41	0.41
11:K:28:ASN:HA	11:K:29:PRO:HD3	1.82	0.41
1:A:1307:U:H5'	13:M:108:THR:HG21	2.01	0.41
17:Q:103:LYS:HZ2	17:Q:103:LYS:HB3	1.83	0.41
18:R:32:THR:HG22	18:R:33:GLY:N	2.36	0.41
19:S:79:TYR:OH	19:S:80:ARG:HD3	2.21	0.41
1:A:163:C:H2'	1:A:164:U:H6	1.85	0.41
1:A:240:C:H2'	1:A:241:C:C6	2.56	0.41
1:A:39:G:H2'	1:A:40:C:H6	1.85	0.41
1:A:41:G:H2'	1:A:42:G:C8	2.56	0.41
1:A:431:A:C2'	1:A:432:A:H5'	2.51	0.41
1:A:685:G:C2	1:A:686:U:C4	3.09	0.41
2:B:128:GLU:C	2:B:130:VAL:H	2.24	0.41
3:C:133:ILE:HG21	3:C:167:ALA:HB3	2.02	0.41
8:H:84:ARG:HH21	8:H:86:ILE:CD1	2.34	0.41
9:I:85:VAL:CG2	9:I:92:ARG:HB3	2.51	0.41
1:A:1201:A:H4'	1:A:1202:G:H5"	2.01	0.41
1:A:1305:G:H5"	21:V:3:GLY:CA	2.44	0.41
1:A:160:A:H1'	1:A:344:A:C5	2.56	0.41
1:A:918:A:H2'	1:A:919:A:O4'	2.21	0.41
2:B:109:LEU:C	2:B:109:LEU:HD23	2.41	0.41
2:B:10:HIS:C	2:B:12:GLY:H	2.23	0.41
2:B:38:LEU:HA	2:B:38:LEU:HD23	1.91	0.41
6:F:40:VAL:HG22	6:F:41:GLU:H	1.86	0.41
1:A:738:C:P	6:F:92:LYS:HZ2	2.44	0.41
8:H:30:ARG:HH11	8:H:30:ARG:HG2	1.85	0.41
14:N:17:VAL:HG23	14:N:18:ARG:H	1.86	0.41
18:R:73:LYS:HD3	18:R:73:LYS:OXT	2.21	0.41
1:A:1469:G:O2'	1:A:1470:G:H5'	2.22	0.40
1:A:15:G:H21	5:E:14:ARG:HA	1.85	0.40
1:A:273:A:H1'	17:Q:15:GLN:OE1	2.21	0.40
1:A:413:G:C2'	1:A:428:G:N2	2.85	0.40
1:A:471:G:H21	16:P:82:GLN:HE21	1.68	0.40
1:A:959:A:O3'	1:A:960:U:H4'	2.22	0.40
2:B:105:ARG:HA	2:B:105:ARG:NE	2.36	0.40
2:B:7:ALA:HA	2:B:11:PHE:CD2	2.56	0.40
3:C:41:LEU:HA	3:C:41:LEU:HD23	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:11:ARG:NH1	5:E:11:ARG:HG3	2.36	0.40
5:E:32:ASP:O	5:E:33:ARG:HB2	2.20	0.40
7:G:49:ILE:O	7:G:53:THR:HB	2.21	0.40
7:G:68:VAL:O	7:G:68:VAL:HG12	2.21	0.40
9:I:43:VAL:CG1	9:I:50:ARG:HH12	2.18	0.40
9:I:92:ARG:HB2	9:I:101:LEU:HD11	2.03	0.40
12:L:31:GLY:HA3	12:L:55:ARG:O	2.21	0.40
13:M:120:LYS:N	13:M:120:LYS:HD2	2.35	0.40
15:O:27:GLN:O	15:O:31:LEU:HB2	2.20	0.40
16:P:43:LYS:HD3	16:P:48:TRP:CE2	2.56	0.40
16:P:82:GLN:O	16:P:83:GLU:C	2.60	0.40
18:R:23:GLU:O	18:R:26:LYS:HE2	2.21	0.40
19:S:41:PRO:C	19:S:43:MET:H	2.25	0.40
20:T:3:LEU:C	20:T:5:ALA:H	2.24	0.40
1:A:1442:G:H2'	1:A:1442(B):A:C8	2.56	0.40
1:A:274:A:O2'	1:A:275:G:C8	2.74	0.40
1:A:334:C:H2'	1:A:335:C:H6	1.85	0.40
1:A:413:G:C2'	1:A:428:G:H22	2.34	0.40
1:A:537:G:H2'	1:A:538:G:H8	1.86	0.40
1:A:624:C:H2'	1:A:625:G:C8	2.57	0.40
1:A:882:C:O2'	1:A:883:C:H5'	2.21	0.40
2:B:126:LYS:H	2:B:126:LYS:HD2	1.85	0.40
3:C:106:GLN:O	3:C:107:ASN:CB	2.68	0.40
3:C:174:LEU:HD21	3:C:200:TYR:HE2	1.84	0.40
3:C:76:ILE:C	3:C:82:ARG:HB3	2.41	0.40
5:E:15:MET:HG3	5:E:16:GLN:H	1.85	0.40
6:F:68:PRO:HB3	6:F:70:ASP:OD1	2.21	0.40
9:I:117:LYS:CG	9:I:120:ARG:HB3	2.51	0.40
11:K:52:GLN:O	11:K:56:LEU:HG	2.22	0.40
13:M:121:LYS:O	13:M:122:ALA:CB	2.68	0.40
13:M:122:ALA:O	13:M:123:PRO:C	2.60	0.40
14:N:28:ARG:HG2	14:N:28:ARG:NH1	2.33	0.40
1:A:1202:G:C2	14:N:41:ILE:HG21	2.56	0.40
1:A:1048:G:N1	1:A:1210:C:N4	2.68	0.40
1:A:1277:C:C3'	1:A:1277:C:C6	3.04	0.40
1:A:240:C:H2'	1:A:241:C:H6	1.86	0.40
2:B:122:GLU:H	2:B:122:GLU:CD	2.24	0.40
2:B:87:VAL:HG11	2:B:91:TRP:CD1	2.55	0.40
4:D:69:ILE:CG2	4:D:73:GLN:HB2	2.51	0.40
5:E:98:ALA:HB1	5:E:102:PRO:HB2	2.03	0.40
10:J:23:GLU:O	10:J:27:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:38:ILE:CD1	11:K:53:LEU:HB3	2.43	0.40
11:K:59:ALA:O	11:K:62:ALA:HB3	2.20	0.40
11:K:99:VAL:HA	18:R:72:ARG:H	1.86	0.40
12:L:113:ARG:O	12:L:115:LYS:O	2.39	0.40
14:N:7:GLU:O	14:N:8:LYS:C	2.60	0.40
19:S:36:ARG:HH11	19:S:36:ARG:CG	2.34	0.40
19:S:4:LEU:O	19:S:5:LYS:HE3	2.22	0.40
1:A:1147:C:O2'	9:I:15:ARG:HG3	2.21	0.40
1:A:407:G:H2'	1:A:408:A:C8	2.56	0.40
1:A:953:G:C5'	1:A:965:A:H61	2.30	0.40
1:A:993:G:C4'	1:A:994:A:OP2	2.65	0.40
2:B:95:MET:O	2:B:99:PHE:HA	2.22	0.40
4:D:152:ARG:HG2	4:D:180:MET:HE1	2.03	0.40
4:D:87:VAL:O	4:D:91:VAL:HG23	2.22	0.40
5:E:2:PHE:HD1	5:E:2:PHE:HA	1.76	0.40
9:I:78:LEU:HD11	9:I:82:ARG:CZ	2.52	0.40
10:J:3:ARG:HH11	10:J:97:LYS:HD3	1.86	0.40
12:L:82:ARG:HB3	12:L:97:VAL:CG2	2.52	0.40
3:C:12:GLY:CA	14:N:56:ARG:CZ	2.98	0.40
17:Q:16:LYS:HA	17:Q:45:ASP:O	2.21	0.40
17:Q:32:GLY:O	17:Q:33:LYS:C	2.59	0.40
19:S:5:LYS:C	19:S:6:LYS:HG3	2.40	0.40
1:A:1201:A:O2'	1:A:1202:G:OP2	2.33	0.40
1:A:1126:U:H6	1:A:1280:A:C5	2.39	0.40
1:A:18:C:O5'	1:A:18:C:H6	2.04	0.40
1:A:564:C:C5	17:Q:30:LEU:HD11	2.57	0.40
1:A:792:A:H4'	1:A:793:U:O5'	2.21	0.40
3:C:29:ARG:NH1	3:C:29:ARG:HG2	2.36	0.40
4:D:35:ARG:HD2	4:D:37:TYR:HE1	1.87	0.40
4:D:7:VAL:O	4:D:9:ARG:N	2.46	0.40
5:E:29:VAL:HG12	5:E:30:VAL:N	2.37	0.40
7:G:114:ARG:HB2	7:G:117:VAL:CG2	2.51	0.40
10:J:58:ARG:O	10:J:59:GLU:CB	2.70	0.40
11:K:116:ARG:O	11:K:117:LYS:CB	2.70	0.40
14:N:17:VAL:HG23	14:N:18:ARG:N	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	233/256 (91%)	168 (72%)	43 (18%)	22 (9%)	0 3
3	C	205/239 (86%)	138 (67%)	37 (18%)	30 (15%)	0 1
4	D	206/208 (99%)	162 (79%)	31 (15%)	13 (6%)	1 9
5	E	149/161 (92%)	129 (87%)	15 (10%)	5 (3%)	3 21
6	F	99/101 (98%)	78 (79%)	19 (19%)	2 (2%)	7 34
7	G	153/155 (99%)	113 (74%)	31 (20%)	9 (6%)	1 11
8	H	136/138 (99%)	111 (82%)	21 (15%)	4 (3%)	4 25
9	I	125/128 (98%)	93 (74%)	19 (15%)	13 (10%)	0 2
10	J	97/104 (93%)	62 (64%)	15 (16%)	20 (21%)	0 0
11	K	117/129 (91%)	95 (81%)	18 (15%)	4 (3%)	3 21
12	L	123/132 (93%)	96 (78%)	17 (14%)	10 (8%)	1 4
13	M	123/126 (98%)	85 (69%)	22 (18%)	16 (13%)	0 1
14	N	58/60 (97%)	36 (62%)	16 (28%)	6 (10%)	0 2
15	O	86/88 (98%)	70 (81%)	14 (16%)	2 (2%)	6 31
16	P	82/88 (93%)	72 (88%)	9 (11%)	1 (1%)	13 46
17	Q	102/104 (98%)	79 (78%)	13 (13%)	10 (10%)	0 3
18	R	71/88 (81%)	57 (80%)	10 (14%)	4 (6%)	2 12
19	S	79/92 (86%)	50 (63%)	19 (24%)	10 (13%)	0 1
20	T	97/106 (92%)	67 (69%)	25 (26%)	5 (5%)	2 13
21	V	23/26 (88%)	16 (70%)	5 (22%)	2 (9%)	1 4
All	All	2364/2529 (94%)	1777 (75%)	399 (17%)	188 (8%)	1 5

All (188) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	3	GLU

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Mol	Chain	Res	Type
2	B	14	GLU
2	B	17	ARG
2	B	18	TRP
2	B	226	PRO
3	C	3	LYS
3	C	14	THR
3	C	25	LYS
3	C	46	LEU
3	C	49	ALA
3	C	100	LEU
3	C	145	ALA
3	C	174	LEU
3	C	188	ALA
3	C	206	VAL
4	D	28	PRO
4	D	35	ARG
4	D	43	GLY
4	D	87	VAL
4	D	128	ASN
4	D	174	SER
5	E	12	THR
6	F	64	GLN
7	G	6	ALA
7	G	154	ARG
8	H	91	ARG
9	I	30	GLN
9	I	42	ALA
9	I	54	ALA
9	I	87	TYR
9	I	116	HIS
10	J	53	LYS
10	J	76	ASN
11	K	116	ARG
12	L	23	LEU
12	L	24	LYS
12	L	26	ALA
12	L	43	LYS
13	M	22	TYR
13	M	26	LYS
13	M	66	GLU
13	M	122	ALA
14	N	3	LYS

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Mol	Chain	Res	Type
14	N	10	LYS
15	O	87	ARG
17	Q	52	LEU
17	Q	98	SER
18	R	72	ARG
19	S	5	LYS
19	S	8	VAL
19	S	80	ARG
20	T	4	SER
20	T	87	ALA
21	V	24	LYS
2	B	15	ARG
2	B	71	ALA
2	B	117	ALA
2	B	159	VAL
2	B	201	ALA
2	B	218	GLN
2	B	222	GLY
3	C	15	ARG
3	C	60	ALA
3	C	75	VAL
3	C	99	ALA
3	C	155	ARG
3	C	180	ASN
4	D	3	TYR
4	D	88	THR
4	D	89	GLY
7	G	80	GLY
8	H	24	THR
8	H	128	GLY
9	I	118	ALA
9	I	126	LYS
10	J	24	ALA
10	J	32	VAL
10	J	34	GLY
10	J	55	LYS
10	J	59	GLU
10	J	70	VAL
10	J	71	ASP
11	K	2	ARG
12	L	44	PRO
13	M	23	GLY

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Mol	Chain	Res	Type
13	M	37	GLY
13	M	62	THR
13	M	67	GLY
13	M	99	GLY
13	M	105	ASN
13	M	123	PRO
14	N	31	SER
16	P	52	ASP
17	Q	79	GLY
18	R	13	GLU
19	S	4	LEU
19	S	13	HIS
19	S	42	GLU
19	S	66	VAL
19	S	67	GLY
20	T	89	GLY
2	B	70	GLN
2	B	143	LEU
2	B	207	LEU
5	E	70	GLY
8	H	22	GLU
9	I	106	ARG
10	J	39	PRO
10	J	90	THR
11	K	3	GLN
12	L	47	ALA
12	L	117	GLY
13	M	20	TYR
13	M	35	LYS
13	M	108	THR
14	N	6	ILE
14	N	9	ALA
14	N	55	VAL
17	Q	29	PRO
17	Q	48	GLU
18	R	11	LEU
19	S	29	LEU
2	B	10	HIS
2	B	124	ARG
2	B	189	ASP
3	C	73	GLY
3	C	80	GLY

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Mol	Chain	Res	Type
3	C	83	ILE
3	C	107	ASN
3	C	143	SER
3	C	167	ALA
3	C	173	PRO
3	C	187	LEU
4	D	25	CYS
4	D	29	LYS
5	E	69	ASN
5	E	136	ARG
7	G	32	ASP
7	G	38	ALA
7	G	111	PRO
9	I	22	ASN
9	I	33	ASN
9	I	92	ARG
10	J	28	SER
10	J	38	LEU
10	J	58	ARG
10	J	88	LEU
11	K	5	ALA
17	Q	73	LEU
20	T	64	THR
20	T	90	ALA
2	B	102	ILE
3	C	74	VAL
3	C	97	ASN
3	C	153	SER
3	C	178	ARG
4	D	170	GLY
5	E	66	PRO
7	G	51	GLU
9	I	23	GLY
9	I	97	PRO
10	J	31	GLN
10	J	37	PRO
12	L	101	TYR
17	Q	80	ARG
17	Q	94	TYR
18	R	5	ALA
21	V	2	LYS
2	B	11	PHE

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Mol	Chain	Res	Type
4	D	4	ILE
7	G	129	GLY
10	J	30	ALA
10	J	79	THR
12	L	83	GLY
17	Q	103	LYS
6	F	96	PRO
19	S	7	GLY
7	G	68	VAL
13	M	5	GLY
10	J	89	PRO
15	O	35	ILE
2	B	121	ILE
3	C	50	GLY
13	M	6	VAL
17	Q	76	VAL
2	B	9	VAL
3	C	204	GLY
12	L	25	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/220 (92%)	180 (89%)	22 (11%)	6	24
3	C	160/188 (85%)	141 (88%)	19 (12%)	5	21
4	D	180/180 (100%)	162 (90%)	18 (10%)	7	28
5	E	115/122 (94%)	100 (87%)	15 (13%)	4	18
6	F	90/90 (100%)	82 (91%)	8 (9%)	9	33
7	G	126/126 (100%)	119 (94%)	7 (6%)	21	53
8	H	119/119 (100%)	111 (93%)	8 (7%)	16	47
9	I	98/99 (99%)	94 (96%)	4 (4%)	30	63
10	J	88/91 (97%)	83 (94%)	5 (6%)	20	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	K	90/99 (91%)	83 (92%)	7 (8%)	12 40
12	L	104/109 (95%)	93 (89%)	11 (11%)	6 25
13	M	100/101 (99%)	93 (93%)	7 (7%)	15 45
14	N	49/49 (100%)	44 (90%)	5 (10%)	7 27
15	O	79/79 (100%)	76 (96%)	3 (4%)	33 65
16	P	72/74 (97%)	67 (93%)	5 (7%)	15 46
17	Q	96/96 (100%)	87 (91%)	9 (9%)	8 30
18	R	64/77 (83%)	59 (92%)	5 (8%)	12 40
19	S	71/79 (90%)	62 (87%)	9 (13%)	4 19
20	T	76/82 (93%)	64 (84%)	12 (16%)	2 11
21	V	19/21 (90%)	18 (95%)	1 (5%)	22 55
All	All	1998/2101 (95%)	1818 (91%)	180 (9%)	9 32

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	2	LYS
2	B	3	GLU
2	B	17	ARG
2	B	18	TRP
2	B	19	ASN
2	B	37	ASP
2	B	61	THR
2	B	76	ARG
2	B	92	LEU
2	B	95	MET
2	B	108	ARG
2	B	111	GLU
2	B	140	GLN
2	B	148	LEU
2	B	159	VAL
2	B	163	LYS
2	B	164	GLU
2	B	172	ARG
2	B	181	LEU
2	B	209	LEU
2	B	218	GLN
2	B	225	GLU

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Mol	Chain	Res	Type
3	C	2	ASN
3	C	3	LYS
3	C	25	LYS
3	C	27	GLN
3	C	32	LEU
3	C	74	VAL
3	C	78	ARG
3	C	94	THR
3	C	126	ARG
3	C	155	ARG
3	C	161	GLN
3	C	165	GLU
3	C	166	TRP
3	C	174	LEU
3	C	176	THR
3	C	189	ARG
3	C	191	THR
3	C	192	TYR
3	C	203	LEU
4	D	2	ARG
4	D	8	CYS
4	D	9	ARG
4	D	28	PRO
4	D	37	TYR
4	D	63	LEU
4	D	79	GLU
4	D	85	LYS
4	D	95	LEU
4	D	113	ARG
4	D	121	ARG
4	D	126	THR
4	D	154	LEU
4	D	155	GLU
4	D	161	LEU
4	D	181	LYS
4	D	193	LEU
4	D	198	ASN
5	E	2	PHE
5	E	8	LEU
5	E	12	THR
5	E	14	ARG
5	E	28	VAL

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Mol	Chain	Res	Type
5	E	37	VAL
5	E	39	LEU
5	E	68	GLN
5	E	75	GLU
5	E	78	VAL
5	E	85	ILE
5	E	123	ASN
5	E	140	THR
5	E	143	ASP
5	E	146	ARG
6	F	10	LEU
6	F	32	ASN
6	F	40	VAL
6	F	45	LEU
6	F	47	ARG
6	F	55	ASP
6	F	67	MET
6	F	86	ARG
7	G	7	GLU
7	G	11	LEU
7	G	12	GLN
7	G	109	GLN
7	G	135	LYS
7	G	137	LYS
7	G	139	ASP
8	H	26	VAL
8	H	50	ARG
8	H	85	ARG
8	H	92	ARG
8	H	95	VAL
8	H	119	LEU
8	H	122	ARG
8	H	127	LEU
9	I	8	ARG
9	I	53	ASP
9	I	126	LYS
9	I	127	ARG
10	J	4	ILE
10	J	19	GLN
10	J	27	ARG
10	J	57	SER
10	J	71	ASP

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Mol	Chain	Res	Type
11	K	17	ASN
11	K	19	ILE
11	K	38	ILE
11	K	44	ARG
11	K	74	VAL
11	K	86	ARG
11	K	96	LYS
12	L	29	ARG
12	L	44	PRO
12	L	49	ARG
12	L	55	ARG
12	L	56	LEU
12	L	63	THR
12	L	81	ILE
12	L	85	ARG
12	L	87	LYS
12	L	109	ARG
12	L	122	LYS
13	M	8	ILE
13	M	13	ARG
13	M	65	LEU
13	M	69	LEU
13	M	109	ARG
13	M	114	LYS
13	M	124	ARG
14	N	7	GLU
14	N	11	ARG
14	N	30	ARG
14	N	31	SER
14	N	43	LEU
15	O	31	LEU
15	O	80	LEU
15	O	87	ARG
16	P	2	VAL
16	P	42	ARG
16	P	45	THR
16	P	53	VAL
16	P	62	VAL
17	Q	21	LEU
17	Q	37	ARG
17	Q	47	GLU
17	Q	54	ASP

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Mol	Chain	Res	Type
17	Q	58	ILE
17	Q	73	LEU
17	Q	76	VAL
17	Q	97	LEU
17	Q	100	ARG
18	R	13	GLU
18	R	17	ARG
18	R	21	ASN
18	R	39	ARG
18	R	72	ARG
19	S	4	LEU
19	S	12	ASP
19	S	19	LEU
19	S	35	ARG
19	S	36	ARG
19	S	61	ILE
19	S	64	ASN
19	S	77	ARG
19	S	80	ARG
20	T	3	LEU
20	T	6	LEU
20	T	18	ARG
20	T	24	SER
20	T	35	GLN
20	T	50	ARG
20	T	55	LEU
20	T	66	HIS
20	T	67	LYS
20	T	68	ASN
20	T	80	LYS
20	T	93	ILE
21	V	14	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	19	ASN
2	B	34	HIS
2	B	72	GLN
2	B	140	GLN
2	B	198	ASN
2	B	218	GLN

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Mol	Chain	Res	Type
2	B	234	GLN
3	C	5	HIS
3	C	30	HIS
3	C	62	ASN
3	C	97	ASN
3	C	106	GLN
3	C	107	ASN
3	C	117	GLN
3	C	180	ASN
4	D	61	GLN
4	D	73	GLN
4	D	160	ASN
4	D	198	ASN
5	E	68	GLN
5	E	69	ASN
5	E	123	ASN
6	F	18	GLN
6	F	27	GLN
6	F	32	ASN
6	F	57	GLN
6	F	64	GLN
6	F	94	GLN
6	F	100	ASN
7	G	85	GLN
7	G	147	ASN
9	I	72	GLN
10	J	54	HIS
10	J	60	HIS
10	J	74	ASN
10	J	76	ASN
11	K	17	ASN
11	K	89	GLN
11	K	107	ASN
12	L	71	HIS
13	M	11	ASN
15	O	61	GLN
16	P	13	HIS
16	P	82	GLN
17	Q	15	GLN
17	Q	95	GLN
18	R	21	ASN
19	S	46	HIS

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Mol	Chain	Res	Type
19	S	56	HIS
19	S	64	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1508/1521 (99%)	247 (16%)	57 (3%)
22	W	3/6 (50%)	0	0
23	Z	15/16 (93%)	2 (13%)	2 (13%)
All	All	1526/1543 (98%)	249 (16%)	59 (3%)

All (249) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	52	G
1	A	60	A
1	A	61	G
1	A	65	U
1	A	66	G
1	A	116	A
1	A	121	C
1	A	131	C
1	A	144	G
1	A	147	G
1	A	149	A
1	A	150	C
1	A	159	G
1	A	160	A
1	A	169	C
1	A	195	A

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Mol	Chain	Res	Type
1	A	196	A
1	A	197	A
1	A	204	U
1	A	217	C
1	A	246	A
1	A	247	G
1	A	250	A
1	A	251	G
1	A	252	U
1	A	266	G
1	A	267	C
1	A	274	A
1	A	275	G
1	A	279	A
1	A	281	G
1	A	282	A
1	A	289	G
1	A	293	G
1	A	304	U
1	A	305	G
1	A	306	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	330	C
1	A	345	C
1	A	352	C
1	A	354	G
1	A	362	G
1	A	367	U
1	A	373	A
1	A	388	G
1	A	403	C
1	A	406	G
1	A	412	A
1	A	414	A
1	A	421	U
1	A	422	C
1	A	423	G
1	A	428	G
1	A	429	U
1	A	439	A

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Mol	Chain	Res	Type
1	A	448	A
1	A	452	A
1	A	453	A
1	A	461	A
1	A	471	G
1	A	485	G
1	A	486	U
1	A	498	U
1	A	500	G
1	A	511	C
1	A	512	U
1	A	516	U
1	A	517	G
1	A	518	C
1	A	524	G
1	A	531	U
1	A	532	A
1	A	533	A
1	A	545	C
1	A	547	A
1	A	548	G
1	A	559	A
1	A	560	U
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	630	G
1	A	648	A
1	A	653	A
1	A	665	A
1	A	687	A
1	A	688	G
1	A	703	G
1	A	721	G
1	A	723	U
1	A	730	G
1	A	731	G
1	A	733	A
1	A	755	G
1	A	777	A
1	A	793	U

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Mol	Chain	Res	Type
1	A	794	A
1	A	815	A
1	A	817	C
1	A	819	A
1	A	821	G
1	A	840	C
1	A	841	U
1	A	848	C
1	A	859	A
1	A	885	G
1	A	889	A
1	A	890	G
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	958	A
1	A	960	U
1	A	968	A
1	A	969	A
1	A	971	G
1	A	976	G
1	A	977	A
1	A	992	U
1	A	993	G
1	A	994	A
1	A	995	C
1	A	998	G
1	A	1001(A)	G
1	A	1004	A
1	A	1021	G
1	A	1024	G
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1030	C
1	A	1046	A
1	A	1048	G
1	A	1050	G
1	A	1054	C
1	A	1055	A

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Mol	Chain	Res	Type
1	A	1065	U
1	A	1068	G
1	A	1070	U
1	A	1081	G
1	A	1084	G
1	A	1085	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1102	A
1	A	1109	C
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1136	U
1	A	1138	G
1	A	1139	G
1	A	1141	C
1	A	1146	A
1	A	1157	A
1	A	1158	C
1	A	1159	U
1	A	1160	G
1	A	1168	A
1	A	1183	A
1	A	1196	U
1	A	1197	G
1	A	1202	G
1	A	1210	C
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1215	G
1	A	1225	A
1	A	1227	A
1	A	1238	A
1	A	1245	A
1	A	1250	A

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Mol	Chain	Res	Type
1	A	1256	A
1	A	1257	U
1	A	1277	C
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1285	A
1	A	1287	A
1	A	1297	C
1	A	1298	C
1	A	1299	A
1	A	1300	G
1	A	1302	U
1	A	1305	G
1	A	1306	A
1	A	1320	C
1	A	1322	C
1	A	1338	G
1	A	1347	G
1	A	1348	U
1	A	1363(A)	A
1	A	1365	G
1	A	1370	G
1	A	1377	A
1	A	1378	C
1	A	1381	U
1	A	1398	A
1	A	1400	C
1	A	1442	G
1	A	1442(B)	A
1	A	1452	C
1	A	1456	G
1	A	1476	G
1	A	1478	C
1	A	1480	G
1	A	1481	U
1	A	1492	A
1	A	1494	G
1	A	1497	G
1	A	1503	A

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Mol	Chain	Res	Type
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1517	G
1	A	1520	G
1	A	1527	C
1	A	1529	G
1	A	1530	G
1	A	1542	U
23	Z	29	G
23	Z	41	C

All (59) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	50	A
1	A	51	A
1	A	65	U
1	A	148	G
1	A	159	G
1	A	196	A
1	A	216	G
1	A	246	A
1	A	250	A
1	A	251	G
1	A	280	C
1	A	281	G
1	A	304	U
1	A	329	A
1	A	344	A
1	A	372	C
1	A	413	G
1	A	428	G
1	A	470	C
1	A	485	G
1	A	496	A
1	A	531	U
1	A	559	A
1	A	572	A
1	A	575	G

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Mol	Chain	Res	Type
1	A	702	A
1	A	730	G
1	A	819	A
1	A	884	U
1	A	968	A
1	A	975	A
1	A	992	U
1	A	993	G
1	A	1054	C
1	A	1084	G
1	A	1101	A
1	A	1135	U
1	A	1145	C
1	A	1157	A
1	A	1182	G
1	A	1201	A
1	A	1210	C
1	A	1214	C
1	A	1282	C
1	A	1297	C
1	A	1305	G
1	A	1319	A
1	A	1335	C
1	A	1347	G
1	A	1377	A
1	A	1397	C
1	A	1442(A)	G
1	A	1447	A
1	A	1452	C
1	A	1480	G
1	A	1504	G
23	Z	28	G
23	Z	40	C

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 182 ligands modelled in this entry, 181 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
26	RPO	A	2800	24	53,53,53	1.41	7 (13%)	73,77,77	1.14	6 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	RPO	A	2800	24	-	9/23/99/99	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	2800	RPO	CAU-CAO	-4.68	1.39	1.50
26	A	2800	RPO	CBI-CBW	3.31	1.61	1.52
26	A	2800	RPO	OAV-CBQ	2.67	1.48	1.41
26	A	2800	RPO	CBC-CAO	2.14	1.43	1.38
26	A	2800	RPO	CAN-CAL	2.12	1.43	1.38
26	A	2800	RPO	CAP-CAN	2.07	1.43	1.38
26	A	2800	RPO	CAM-CAO	2.03	1.43	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	2800	RPO	O1'-C1'-O4'	-4.70	106.35	111.43
26	A	2800	RPO	O4-CAU-CAO	2.96	116.73	109.91
26	A	2800	RPO	OAV-CBM-CAQ	2.88	111.37	106.01
26	A	2800	RPO	O1'-CBW-CBI	2.33	113.47	107.28
26	A	2800	RPO	CAQ-CBM-CBJ	-2.14	108.90	113.10
26	A	2800	RPO	CBI-CBW-CBT	-2.04	106.99	111.66

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	A	2800	RPO	NAA-CAQ-CBM-OAV
26	A	2800	RPO	O5-C5-C6-O6
26	A	2800	RPO	C4-C5-C6-O6
26	A	2800	RPO	CBT-CBW-O1'-C1'
26	A	2800	RPO	CBI-CBW-O1'-C1'
26	A	2800	RPO	OAV-CBQ-O3'-C3'
26	A	2800	RPO	O4'-C1'-O1'-CBW
26	A	2800	RPO	C2'-C1'-O1'-CBW
26	A	2800	RPO	CBW-CBT-O1-C1

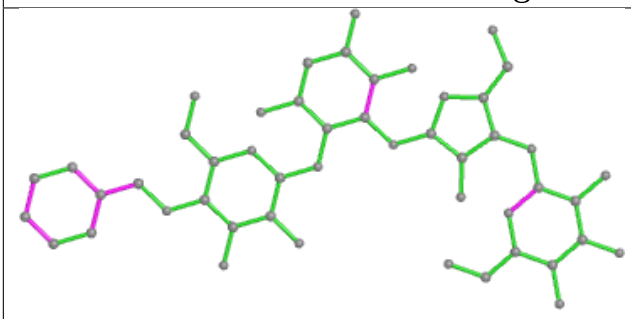
There are no ring outliers.

1 monomer is involved in 6 short contacts:

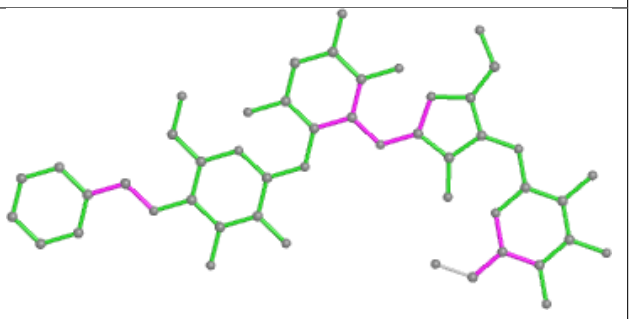
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	2800	RPO	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

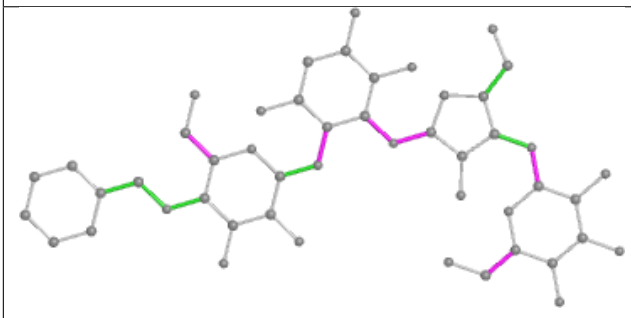
Ligand RPO A 2800



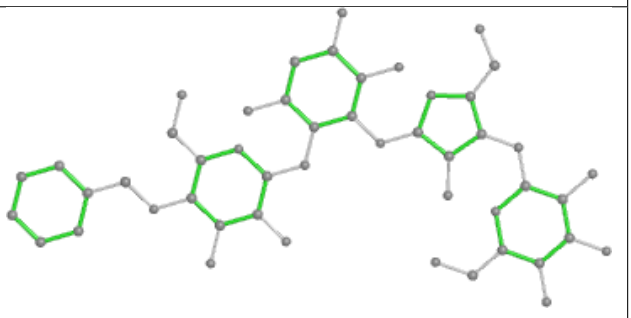
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1510/1521 (99%)	-0.16	8 (0%) 91 86	42, 70, 136, 190	0
2	B	235/256 (91%)	-0.09	7 (2%) 50 33	50, 100, 157, 197	0
3	C	207/239 (86%)	-0.22	0 100 100	50, 90, 137, 169	0
4	D	208/208 (100%)	-0.17	6 (2%) 51 35	49, 83, 134, 196	0
5	E	151/161 (93%)	-0.40	0 100 100	38, 62, 102, 160	0
6	F	101/101 (100%)	-0.23	0 100 100	61, 96, 126, 150	0
7	G	155/155 (100%)	-0.27	4 (2%) 56 40	51, 89, 149, 183	0
8	H	138/138 (100%)	-0.55	0 100 100	36, 60, 90, 112	0
9	I	127/128 (99%)	-0.09	1 (0%) 86 78	42, 102, 138, 201	0
10	J	99/104 (95%)	0.51	9 (9%) 9 5	51, 118, 178, 201	0
11	K	119/129 (92%)	-0.06	3 (2%) 57 42	44, 72, 122, 182	0
12	L	125/132 (94%)	-0.18	4 (3%) 47 30	37, 67, 122, 184	0
13	M	125/126 (99%)	0.52	13 (10%) 6 3	52, 86, 152, 201	0
14	N	60/60 (100%)	-0.15	0 100 100	46, 82, 104, 173	0
15	O	88/88 (100%)	-0.23	1 (1%) 80 70	43, 75, 115, 170	0
16	P	84/88 (95%)	-0.36	0 100 100	45, 64, 94, 172	0
17	Q	104/104 (100%)	0.05	5 (4%) 30 17	37, 68, 136, 201	0
18	R	73/88 (82%)	-0.19	2 (2%) 54 38	55, 82, 145, 179	0
19	S	81/92 (88%)	-0.05	1 (1%) 79 68	67, 100, 150, 166	0
20	T	99/106 (93%)	-0.31	0 100 100	40, 68, 116, 176	0
21	V	25/26 (96%)	0.41	2 (8%) 12 6	51, 73, 121, 144	0
22	W	4/6 (66%)	0.32	0 100 100	86, 89, 91, 91	0
23	Z	15/16 (93%)	0.45	0 100 100	74, 107, 185, 189	0
All	All	3933/4072 (96%)	-0.14	66 (1%) 70 57	36, 76, 142, 201	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	122	ALA	20.8
11	K	119	SER	11.6
17	Q	104	ALA	11.3
13	M	123	PRO	11.1
17	Q	102	GLY	10.9
13	M	120	LYS	10.7
13	M	119	LYS	8.6
13	M	121	LYS	7.1
17	Q	101	GLY	6.6
13	M	125	LYS	6.4
17	Q	103	LYS	6.0
2	B	125	PRO	5.8
21	V	25	LYS	5.7
11	K	118	ALA	5.7
13	M	6	VAL	5.6
13	M	124	ARG	5.4
13	M	118	GLY	5.0
4	D	36	PRO	4.7
4	D	34	ARG	4.7
10	J	34	GLY	4.4
19	S	2	ARG	4.1
1	A	630	G	4.1
12	L	124	ALA	4.0
4	D	22	GLY	4.0
10	J	32	VAL	3.8
1	A	1001(A)	G	3.6
17	Q	100	ARG	3.5
1	A	1129	C	3.5
13	M	1	ALA	3.2
10	J	33	SER	3.2
18	R	1	PRO	3.2
21	V	24	LYS	3.2
11	K	117	LYS	3.1
10	J	31	GLN	3.1
4	D	44	GLN	3.0
10	J	83	LEU	2.9
12	L	15	ARG	2.9
4	D	35	ARG	2.8
2	B	128	GLU	2.8
1	A	723	U	2.8
1	A	1003	G	2.7
2	B	124	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
12	L	123	GLU	2.7
7	G	80	GLY	2.7
2	B	115	LEU	2.6
2	B	127	LYS	2.6
2	B	126	LYS	2.6
1	A	1533	C	2.5
10	J	73	ILE	2.5
15	O	88	GLY	2.5
7	G	81	GLY	2.4
13	M	117	ALA	2.4
10	J	70	VAL	2.4
12	L	125	ALA	2.3
4	D	41	GLN	2.3
13	M	116	VAL	2.3
7	G	84	TYR	2.3
10	J	3	ARG	2.2
1	A	1031	G	2.1
10	J	15	ASP	2.1
18	R	2	SER	2.1
7	G	155	TRP	2.1
1	A	1131	G	2.1
2	B	223	VAL	2.1
9	I	127	ARG	2.0
13	M	10	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	2608	1/1	-0.01	0.48	82,82,82,82	0
24	MG	A	2551	1/1	0.49	0.26	81,81,81,81	0
24	MG	A	2554	1/1	0.51	0.68	82,82,82,82	0
24	MG	A	2636	1/1	0.53	0.30	68,68,68,68	0
24	MG	A	2690	1/1	0.55	0.35	80,80,80,80	0
24	MG	A	2606	1/1	0.55	0.20	69,69,69,69	0
24	MG	A	2662	1/1	0.58	0.53	89,89,89,89	0
24	MG	L	1125	1/1	0.61	0.51	84,84,84,84	0
24	MG	A	2697	1/1	0.63	0.53	86,86,86,86	0
24	MG	A	2618	1/1	0.64	0.28	61,61,61,61	0
24	MG	A	2663	1/1	0.64	0.54	58,58,58,58	0
24	MG	A	2597	1/1	0.67	0.43	62,62,62,62	0
24	MG	A	2626	1/1	0.67	0.69	61,61,61,61	0
25	K	A	2673	1/1	0.70	0.38	105,105,105,105	0
24	MG	A	2687	1/1	0.70	0.39	65,65,65,65	0
25	K	A	2676	1/1	0.71	0.39	111,111,111,111	0
24	MG	A	2686	1/1	0.72	0.25	75,75,75,75	0
25	K	A	2681	1/1	0.72	0.19	87,87,87,87	0
25	K	A	2680	1/1	0.73	0.56	114,114,114,114	0
24	MG	A	2552	1/1	0.74	0.98	58,58,58,58	0
24	MG	A	2660	1/1	0.74	0.16	49,49,49,49	0
24	MG	A	2596	1/1	0.74	0.33	90,90,90,90	0
24	MG	A	2649	1/1	0.76	0.24	48,48,48,48	0
24	MG	A	2631	1/1	0.76	0.48	64,64,64,64	0
24	MG	A	2601	1/1	0.76	0.14	36,36,36,36	0
24	MG	A	2550	1/1	0.77	0.20	50,50,50,50	0
24	MG	A	2645	1/1	0.77	0.44	76,76,76,76	0
24	MG	A	2585	1/1	0.77	0.27	73,73,73,73	0
24	MG	A	2700	1/1	0.78	0.47	69,69,69,69	0
24	MG	A	2668	1/1	0.78	0.27	60,60,60,60	0
24	MG	H	1139	1/1	0.78	0.22	56,56,56,56	0
24	MG	A	2622	1/1	0.79	0.24	50,50,50,50	0
24	MG	A	2549	1/1	0.79	0.17	55,55,55,55	0
24	MG	A	2666	1/1	0.79	0.24	68,68,68,68	0
24	MG	A	2661	1/1	0.79	0.27	67,67,67,67	0
24	MG	A	2570	1/1	0.79	0.19	89,89,89,89	0
24	MG	A	2545	1/1	0.79	0.11	58,58,58,58	0
25	K	A	2678	1/1	0.80	0.21	108,108,108,108	0
24	MG	A	2627	1/1	0.80	0.26	56,56,56,56	0
24	MG	A	2640	1/1	0.80	0.28	55,55,55,55	0
24	MG	A	2568	1/1	0.80	0.20	66,66,66,66	0
24	MG	A	2613	1/1	0.80	0.58	50,50,50,50	0
24	MG	A	2652	1/1	0.80	0.18	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	K	A	2675	1/1	0.81	0.18	97,97,97,97	0
24	MG	A	2692	1/1	0.81	0.64	55,55,55,55	0
24	MG	A	2638	1/1	0.81	0.32	64,64,64,64	0
24	MG	A	2548	1/1	0.81	0.61	70,70,70,70	0
25	K	A	2679	1/1	0.81	0.21	85,85,85,85	0
24	MG	A	2619	1/1	0.82	0.41	83,83,83,83	0
24	MG	A	2572	1/1	0.82	0.21	32,32,32,32	0
24	MG	A	2695	1/1	0.82	0.33	66,66,66,66	0
24	MG	A	2685	1/1	0.82	0.20	45,45,45,45	0
25	K	A	2683	1/1	0.82	0.22	110,110,110,110	0
24	MG	A	2590	1/1	0.82	0.46	56,56,56,56	0
24	MG	A	2689	1/1	0.83	0.42	49,49,49,49	0
24	MG	A	2669	1/1	0.83	0.43	70,70,70,70	0
24	MG	A	2694	1/1	0.83	0.46	68,68,68,68	0
24	MG	A	2559	1/1	0.83	0.38	51,51,51,51	0
24	MG	A	2635	1/1	0.83	0.30	57,57,57,57	0
24	MG	E	1151	1/1	0.83	0.39	55,55,55,55	0
24	MG	A	2609	1/1	0.84	0.70	57,57,57,57	0
24	MG	A	2710	1/1	0.84	0.78	81,81,81,81	0
24	MG	A	2577	1/1	0.84	0.26	50,50,50,50	0
24	MG	A	2566	1/1	0.84	0.53	55,55,55,55	0
24	MG	A	2629	1/1	0.84	0.23	58,58,58,58	0
24	MG	A	2605	1/1	0.84	0.59	50,50,50,50	0
24	MG	A	2651	1/1	0.85	0.33	58,58,58,58	0
24	MG	A	2667	1/1	0.85	0.37	57,57,57,57	0
24	MG	K	1121	1/1	0.86	0.30	43,43,43,43	0
25	K	A	2671	1/1	0.86	0.12	93,93,93,93	0
25	K	A	2682	1/1	0.86	0.22	107,107,107,107	0
24	MG	A	2656	1/1	0.86	0.64	77,77,77,77	0
24	MG	A	2639	1/1	0.86	0.15	48,48,48,48	0
24	MG	A	2592	1/1	0.86	0.63	81,81,81,81	0
24	MG	A	2617	1/1	0.87	0.17	47,47,47,47	0
24	MG	A	2646	1/1	0.87	0.19	46,46,46,46	0
24	MG	A	2653	1/1	0.87	0.17	57,57,57,57	0
24	MG	A	2655	1/1	0.87	0.16	56,56,56,56	0
24	MG	A	2594	1/1	0.88	0.23	39,39,39,39	0
24	MG	A	2557	1/1	0.88	0.38	118,118,118,118	0
24	MG	A	2573	1/1	0.88	0.39	51,51,51,51	0
24	MG	A	2547	1/1	0.88	0.35	14,14,14,14	0
25	K	A	2672	1/1	0.88	0.15	100,100,100,100	0
24	MG	A	2632	1/1	0.88	0.17	75,75,75,75	0
24	MG	A	2574	1/1	0.88	0.41	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	2602	1/1	0.88	0.51	60,60,60,60	0
24	MG	F	1102	1/1	0.88	0.13	61,61,61,61	0
24	MG	A	2567	1/1	0.89	0.36	38,38,38,38	0
24	MG	A	2621	1/1	0.89	0.17	70,70,70,70	0
24	MG	A	2670	1/1	0.89	0.21	57,57,57,57	0
24	MG	A	2589	1/1	0.89	0.22	38,38,38,38	0
24	MG	A	2706	1/1	0.89	0.61	57,57,57,57	0
24	MG	M	1126	1/1	0.90	0.12	57,57,57,57	0
24	MG	A	2642	1/1	0.90	0.17	47,47,47,47	0
24	MG	A	2628	1/1	0.90	0.13	42,42,42,42	0
24	MG	A	2650	1/1	0.90	0.17	32,32,32,32	0
24	MG	T	1100	1/1	0.90	0.32	51,51,51,51	0
24	MG	A	2633	1/1	0.90	0.19	51,51,51,51	0
24	MG	A	2705	1/1	0.90	0.11	59,59,59,59	0
24	MG	A	2604	1/1	0.90	0.28	51,51,51,51	0
24	MG	A	2615	1/1	0.90	0.16	37,37,37,37	0
24	MG	A	2709	1/1	0.90	0.69	95,95,95,95	0
24	MG	A	2561	1/1	0.91	0.29	44,44,44,44	0
24	MG	A	2664	1/1	0.91	0.27	47,47,47,47	0
24	MG	A	2587	1/1	0.91	0.54	40,40,40,40	0
24	MG	A	2707	1/1	0.91	0.27	51,51,51,51	0
24	MG	A	2658	1/1	0.91	0.07	72,72,72,72	0
24	MG	A	2571	1/1	0.91	0.68	53,53,53,53	0
24	MG	A	2684	1/1	0.91	0.56	65,65,65,65	0
24	MG	A	2607	1/1	0.91	0.54	56,56,56,56	0
25	K	A	2677	1/1	0.91	0.13	98,98,98,98	0
24	MG	A	2612	1/1	0.91	0.22	40,40,40,40	0
24	MG	A	2623	1/1	0.92	0.28	48,48,48,48	0
24	MG	A	2560	1/1	0.92	0.52	45,45,45,45	0
24	MG	A	2558	1/1	0.92	0.20	69,69,69,69	0
24	MG	B	1235	1/1	0.92	0.33	66,66,66,66	0
24	MG	A	2644	1/1	0.93	0.07	35,35,35,35	0
24	MG	A	2634	1/1	0.93	0.13	45,45,45,45	0
24	MG	A	2553	1/1	0.93	0.21	58,58,58,58	0
24	MG	A	2665	1/1	0.93	0.25	52,52,52,52	0
24	MG	A	2578	1/1	0.93	0.38	43,43,43,43	0
24	MG	A	2713	1/1	0.93	0.20	75,75,75,75	0
24	MG	A	2556	1/1	0.93	0.65	49,49,49,49	0
24	MG	A	2704	1/1	0.93	0.34	63,63,63,63	0
24	MG	A	2648	1/1	0.93	0.35	35,35,35,35	0
24	MG	A	2630	1/1	0.93	0.13	39,39,39,39	0
24	MG	A	2581	1/1	0.93	0.24	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	2703	1/1	0.93	0.62	59,59,59,59	0
24	MG	A	2616	1/1	0.93	0.58	54,54,54,54	0
26	RPO	A	2800	49/49	0.93	0.21	51,58,75,76	0
24	MG	A	2582	1/1	0.94	0.57	39,39,39,39	0
24	MG	A	2591	1/1	0.94	0.23	53,53,53,53	0
24	MG	A	2688	1/1	0.94	0.13	44,44,44,44	0
24	MG	A	2599	1/1	0.94	0.20	75,75,75,75	0
24	MG	A	2579	1/1	0.94	0.26	38,38,38,38	0
24	MG	A	2569	1/1	0.94	0.11	48,48,48,48	0
24	MG	A	2546	1/1	0.94	0.42	29,29,29,29	0
24	MG	A	2714	1/1	0.94	0.38	64,64,64,64	0
24	MG	A	2575	1/1	0.94	0.31	40,40,40,40	0
24	MG	A	2588	1/1	0.94	0.23	36,36,36,36	0
25	K	A	2674	1/1	0.94	0.30	91,91,91,91	0
24	MG	A	2712	1/1	0.94	0.47	49,49,49,49	0
24	MG	A	2611	1/1	0.95	0.43	38,38,38,38	0
24	MG	L	1126	1/1	0.95	0.20	47,47,47,47	0
24	MG	K	1120	1/1	0.95	0.09	46,46,46,46	0
24	MG	A	2624	1/1	0.95	0.06	40,40,40,40	0
24	MG	A	2586	1/1	0.95	0.11	46,46,46,46	0
24	MG	A	2711	1/1	0.96	0.82	50,50,50,50	0
24	MG	A	2654	1/1	0.96	0.31	95,95,95,95	0
24	MG	A	2555	1/1	0.96	0.37	32,32,32,32	0
24	MG	A	2659	1/1	0.96	0.18	31,31,31,31	0
24	MG	A	2696	1/1	0.96	0.09	43,43,43,43	0
24	MG	A	2583	1/1	0.96	0.18	52,52,52,52	0
24	MG	A	2614	1/1	0.96	0.17	46,46,46,46	0
24	MG	A	2565	1/1	0.96	0.43	37,37,37,37	0
24	MG	A	2625	1/1	0.96	0.08	42,42,42,42	0
24	MG	A	2698	1/1	0.96	0.61	56,56,56,56	0
24	MG	A	2600	1/1	0.96	0.57	53,53,53,53	0
24	MG	A	2593	1/1	0.96	0.25	31,31,31,31	0
24	MG	A	2701	1/1	0.97	0.58	65,65,65,65	0
24	MG	A	2637	1/1	0.97	0.80	78,78,78,78	0
24	MG	A	2580	1/1	0.97	0.35	37,37,37,37	0
24	MG	A	2603	1/1	0.97	0.22	18,18,18,18	0
24	MG	A	2595	1/1	0.97	0.41	55,55,55,55	0
24	MG	A	2620	1/1	0.97	0.18	56,56,56,56	0
27	ZN	D	1209	1/1	0.97	0.21	107,107,107,107	0
24	MG	A	2562	1/1	0.97	0.31	44,44,44,44	0
24	MG	A	2564	1/1	0.97	0.36	41,41,41,41	0
24	MG	A	2576	1/1	0.97	0.30	37,37,37,37	0

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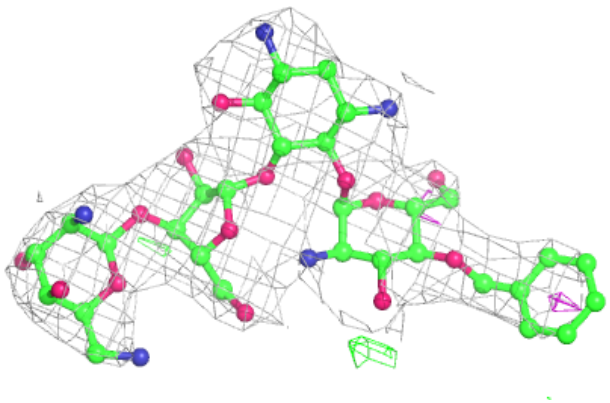
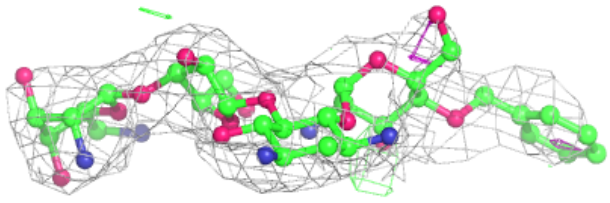
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	2610	1/1	0.97	0.17	42,42,42,42	0
24	MG	A	2702	1/1	0.97	0.44	46,46,46,46	0
24	MG	A	2691	1/1	0.98	0.11	57,57,57,57	0
24	MG	A	2598	1/1	0.98	0.62	38,38,38,38	0
24	MG	A	2708	1/1	0.98	0.60	57,57,57,57	0
24	MG	A	2584	1/1	0.98	0.27	56,56,56,56	0
24	MG	A	2693	1/1	0.98	0.12	64,64,64,64	0
24	MG	A	2647	1/1	0.98	0.13	45,45,45,45	0
27	ZN	N	1061	1/1	0.99	0.16	160,160,160,160	0
24	MG	A	2563	1/1	0.99	0.28	37,37,37,37	0
24	MG	A	2657	1/1	0.99	0.13	55,55,55,55	0
24	MG	A	2641	1/1	0.99	0.35	35,35,35,35	0
24	MG	A	2643	1/1	0.99	0.15	32,32,32,32	0

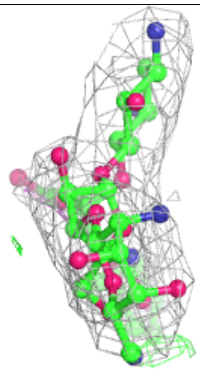
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around RPO A 2800:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.